

AD-A008 035

A HIGH ALTITUDE INFRARED RADIANCE MODEL

Thomas C. Degges

Visidyne, Incorporated

Prepared for:

Air Force Cambridge Research Laboratories
Defense Advanced Research Projects

27 December 1974

DISTRIBUTED BY:

NTIS

National Technical Information Service
U. S. DEPARTMENT OF COMMERCE

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER AFCRL-TR-74-0606	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER AD-A008 035
4. TITLE (and Subtitle) A HIGH ALTITUDE INFRARED RADIANCE MODEL		5. TYPE OF REPORT & PERIOD COVERED Final, 1 June 1972 through 30 April 1974
		6. PERFORMING ORG. REPORT NUMBER VI-236
7. AUTHOR(s) Thomas C. Degges		8. CONTRACT OR GRANT NUMBER(s) F19628-72-C-0330
9. PERFORMING ORGANIZATION NAME AND ADDRESS Visidyne, Inc. 19 Third Avenue, N.W. Industrial Park Burlington, Massachusetts 01803		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 8692 N/A N/A
11. CONTROLLING OFFICE NAME AND ADDRESS Air Force Cambridge Research Laboratories Hanscom AFB, Massachusetts 01731 Contract Monitor: Bertram D. Schurin/OPI		12. REPORT DATE December 27, 1974
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		13. NUMBER OF PAGES 346
		15. SECURITY CLASS. (of this report) Unclassified
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report) Approved for public release; distribution unlimited		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report) Reproduced by NATIONAL TECHNICAL INFORMATION SERVICE US Department of Commerce Springfield, VA. 22151 PRICES SUBJECT TO CHANGE		
18. SUPPLEMENTARY NOTES This research was sponsored by Defense Advanced Research Projects Agency. ARPA Order No. 1366		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Atmosphere, Infrared, Radiance, Model		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) A knowledge of the natural infrared radiance originating in the earth's upper atmosphere is of interest for systems design, military surveillance and the advancement of knowledge about physical pro- cesses in the upper atmosphere. A physical model that includes experimental data on and theoretical estimates of excitation processes that lead to emission of infrared radiation has been implemented in a		

DD FORM 1 JAN 73 1473

EDITION OF 1 NOV 65 IS OBSOLETE

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

20. computer program that computes infrared radiances for an earth limb viewing geometry. The nominal spectral region of this study lies between 2.7 and 25 micrometers and emphasis is placed on radiation originating at altitudes between 70 and 500 km. The physical model is described, with emphasis on the changes required in extending its usefulness. Application of the computer program is described and estimates are given of uncertainties in results due to assumptions made in the model and lack of data on actual atmospheric composition.

Unclassified

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

TABLE OF CONTENTS

<u>SECTION</u>		<u>Page No.</u>
I	Introduction	1
II	Radiative Processes and Modelling	5
III	Atmospheric Composition	39
IV	Results from Computational Model	55
V	High Altitude Radiance Programs	77
	References	261
APPENDIX	Chemistry Program SNAPS2	273

SECTION I

INTRODUCTION

The research reported here has had as its major objective the development of a computer program to simulate the natural infrared radiance background of the earth's upper atmosphere. The nominal spectral region under study lies between 2.7 and 25 micrometers and emphasis is placed on radiation originating at altitudes between 70 and 500 kilometers. The general problem area is of interest for systems design, military surveillance and the advancement of knowledge about physical processes in the upper atmosphere. The immediate application of this work will be to aid in developing optimum infrared background measurements programs and in interpreting the results of such measurements.

This work is an extension of the study of Corbin, et al. (1969) and Degges (1972). The former investigated the natural infrared background of the earth in the 5 to 25 micrometer spectral region, with the goal of estimating earth limb viewing radiances for tangent heights from the surface to 500 km altitude. For convenience, their study divided the atmosphere into two regions with a division at 70 km. Below 70 km the atmosphere was assumed to be in thermal equilibrium. Above 70 km explicit calculations were made of processes which excite and de-excite molecular vibrational and rotational levels which are the source of infrared radiation. Their study concentrated on radiation from water vapor, carbon dioxide, ozone, nitric oxide and nitrous oxide, which are the principal radiating species in the

spectral region considered. In addition, nitric acid was included in the lower atmosphere work and estimates were made of radiation to be expected from particulate matter suspended in the atmosphere.

Corbin, et al. (1969) presented models for the lower atmosphere for a wide range of seasonal and latitudinal conditions. This was not possible for the abundances of most minor neutral species. More data has since become available, particularly for nitric oxide and the hydroxyl radical, but at present it appears that the best means of estimating abundances of important infrared emitting species is chemical rate equation integrations including molecular diffusion and eddy mixing. Even calculations involving transport properties cannot always be accepted because the values of eddy mixing coefficients are to a large extent only informed guesses and published calculations often use outdated rate coefficients. Degges (1972) reported a computer program with which to determine diurnal variations in abundances of minor species, to investigate the effects of changes in assumed eddy mixing coefficients, and to estimate the effects of new determinations of chemical rate coefficients.

A second area of study involved in improving the radiance model includes the physical processes that control the population of infrared emitting states of atmospheric molecules. Except for the pure rotational radiation from molecules such as water, the degree of excitation of vibrational levels determines the radiation from infrared emitting molecules. The most important mechanisms are collisional excitation and de-excitation and absorption and re-emission of electromagnetic radiation.

In the troposphere and lower stratosphere, collisional processes are rapid enough to control the population of vibrational levels.

Above 30 to 50 km, however, collisional excitation becomes less efficient and radiative processes become important. The combined effects of collisional and radiative processes must therefore be considered. Below an altitude of about 90 km molecular nitrogen and oxygen are the most important collision partners. Above that altitude, atomic oxygen becomes important, both in exciting nitric oxide and in determining molecular oxygen and nitrogen vibrational temperatures.

In determining the effects of radiation on the populations of vibrational levels of infrared active molecules, it is necessary to separate the radiation of a single change in vibrational quantum numbers from the rest of the radiation field. The previously reported studies did this by assuming a Doppler line shape for the individual rotational lines of a band and were able to obtain adequate numerical approximations for radiative transfer functions appropriate to single bands of linear molecules, and less accurately, for water vapor and ozone bands lying in the spectral region of interest.

The principal areas of research and program revision reported here include a further study of band radiance modeling and the effects of line shape on radiance computations. In addition to some exploratory calculations using a Voigt line profile instead of a Doppler line shape, some asymptotic analytical results have been obtained which provide an estimate of the accuracy of the numerically obtained band functions at large optical thicknesses. It is found that when a Voigt profile is used, the connection between the band models and functions for a single line is more readily seen than when a Doppler line shape is used. This material, and a discussion of changes made in the numerical methods is described in Section II.

The status of current knowledge of atmospheric composition is reviewed in Section III. Recent measurements of chemical rate coefficients have resulted in changes in estimates of abundances of some molecular species. An attempt is made to set upper and lower bounds for mixing ratios at high altitudes.

Results of calculations are given in Section IV, and estimates are made of the validity of the results.

The computer programs are described in Section V.

SECTION II

RADIATIVE PROCESSES AND MODELLING

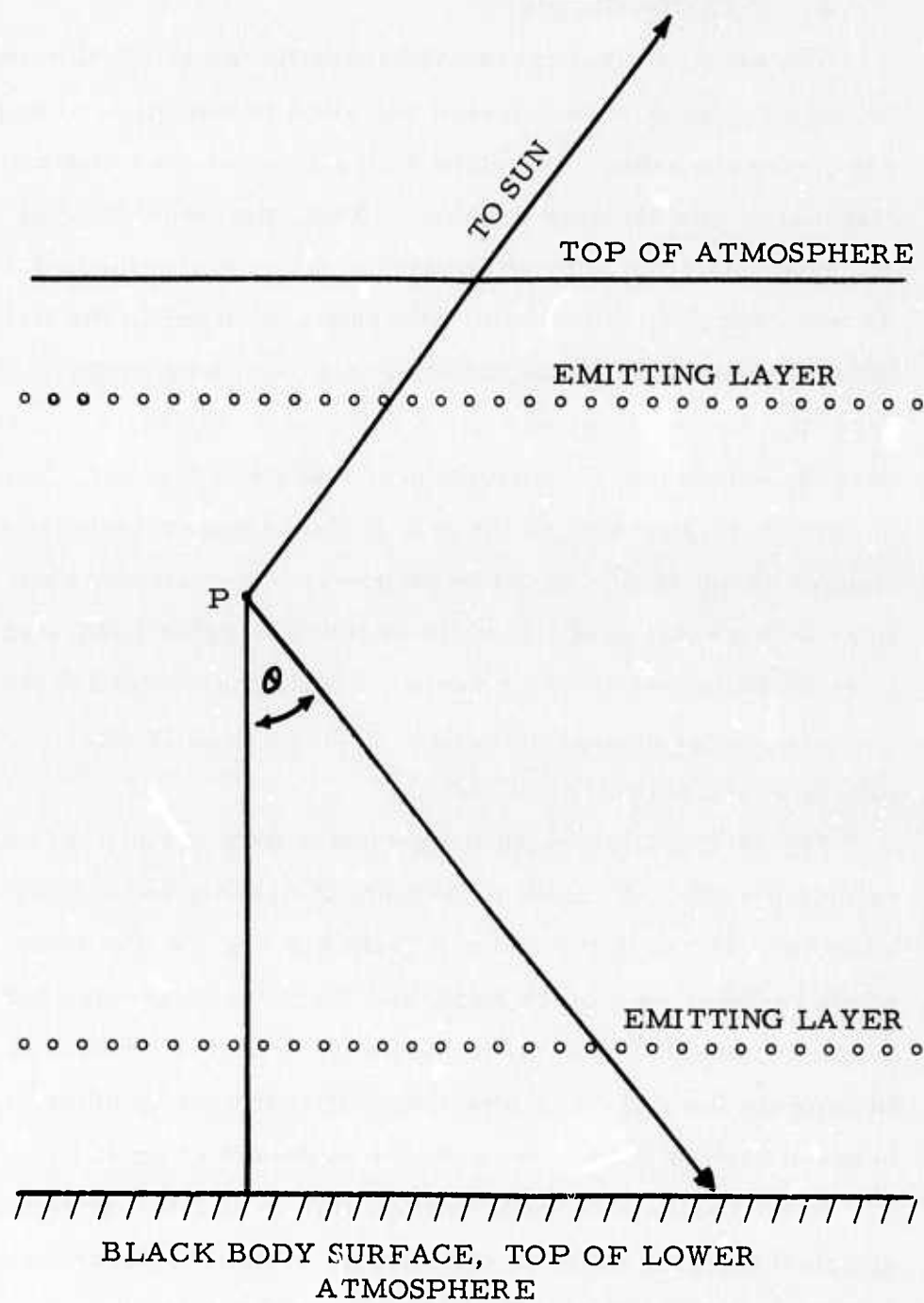
A. INTRODUCTION

The physical processes and assumptions used in developing a model for transport of infrared radiation in the upper atmosphere are discussed below, beginning with a general overview and discussion of a simpler problem. Next, the interaction of electromagnetic radiation with an isolated atom or molecule is described. An understanding of the basic processes involved is the first step in any computation of the radiation from a gas or mixture of gases. Subsequently, absorption from a continuum source, a spectrally varying source and fluorescent processes are treated. The effects of optical thickness when the path of the radiation includes a large number of molecules of the same species is considered for spectral lines with a Voigt profile, which includes Doppler (Gaussian) and Lorentz shapes as limiting cases. Finally, a model for the transport of radiation for a single vibration-rotation band is described, and the effects of temperature estimated.

Figure II-1 illustrates the geometry employed in the current modeling study. A molecule at point P absorbs radiation from three sources; (1) a collimated beam from the sun, (2) the lower boundary which radiates as a black body, and (3) other molecules between the lower and upper boundaries. Radiative transfer functions are needed to compute the effects of absorption of radiation by other molecules between each of the sources and the molecule at point P.

In the absence of collisional excitation and de-excitation, the simplest integral equation that may be written to describe radiative transport in a finite plane parallel atmosphere is

$$J(\tau) = \frac{1}{2} \int_0^{\tau_{\max}} K_1(|\tau - t|) J(t) dt + S(\tau) \quad (2-1)$$



Geometry assumed in deriving the radiative transfer functions

FIGURE II-1

This equation assumes that there is only one radiative transition involved and that the radiation emitted by a molecule after absorption is independent of the direction of incidence. Here τ is a measure of the optical path length in the vertical direction. $J(\tau)$ is a dimensionless measure of the population of the upper, emitting molecular state. $K_1(\tau)$ is the radiative transfer function which accounts for absorption of radiation emitted by molecules at a vertical path length τ distant from the absorbing molecule. $S(\tau)$ is an auxiliary function which includes the effects of radiation originating outside the atmosphere. If there is only a black body source located at the lower boundary from which optical path length is measured ($\tau = 0$ at the lower boundary) then

$$S(\tau) = \frac{1}{2} N_0 K_2(\tau) \quad (2-2)$$

Here N_0 is the radiance of the lower boundary in arbitrary units such as $\text{watts cm}^{-2} \text{ - ster}^{-1}$ or the spectral radiance in units such as $\text{watts cm}^{-2} \text{ cm}^{-2} \text{ - ster}^{-1} (\text{wavelength interval})^{-1}$.

In the gray or spectrally independent case, when equation (2-2) holds, the kernel function $K_1(\tau)$ is the first exponential integral $E_1(\tau)$ and the function describing absorption from the black body source is the second exponential integral $E_2(\tau)$. These functions are described in detail in such works as Kourganoff (1963). A complete analytic solution is available and the auxiliary functions required for a numerical solution have been tabulated by King (1956). Figure (2-2) plots the solution of equation (2-1) when equation (2-2) holds for the gray case for values of total optical thickness $\tau_{\text{max}} = 0, 0.1, 1.0, \text{ and } 10$. When the total optical thickness is small, the

Effect of Optical Thickness on Relative Vibrational
Excitation of Atmosphere Illuminated From Below
By Black Body Source.
[Gray Case]

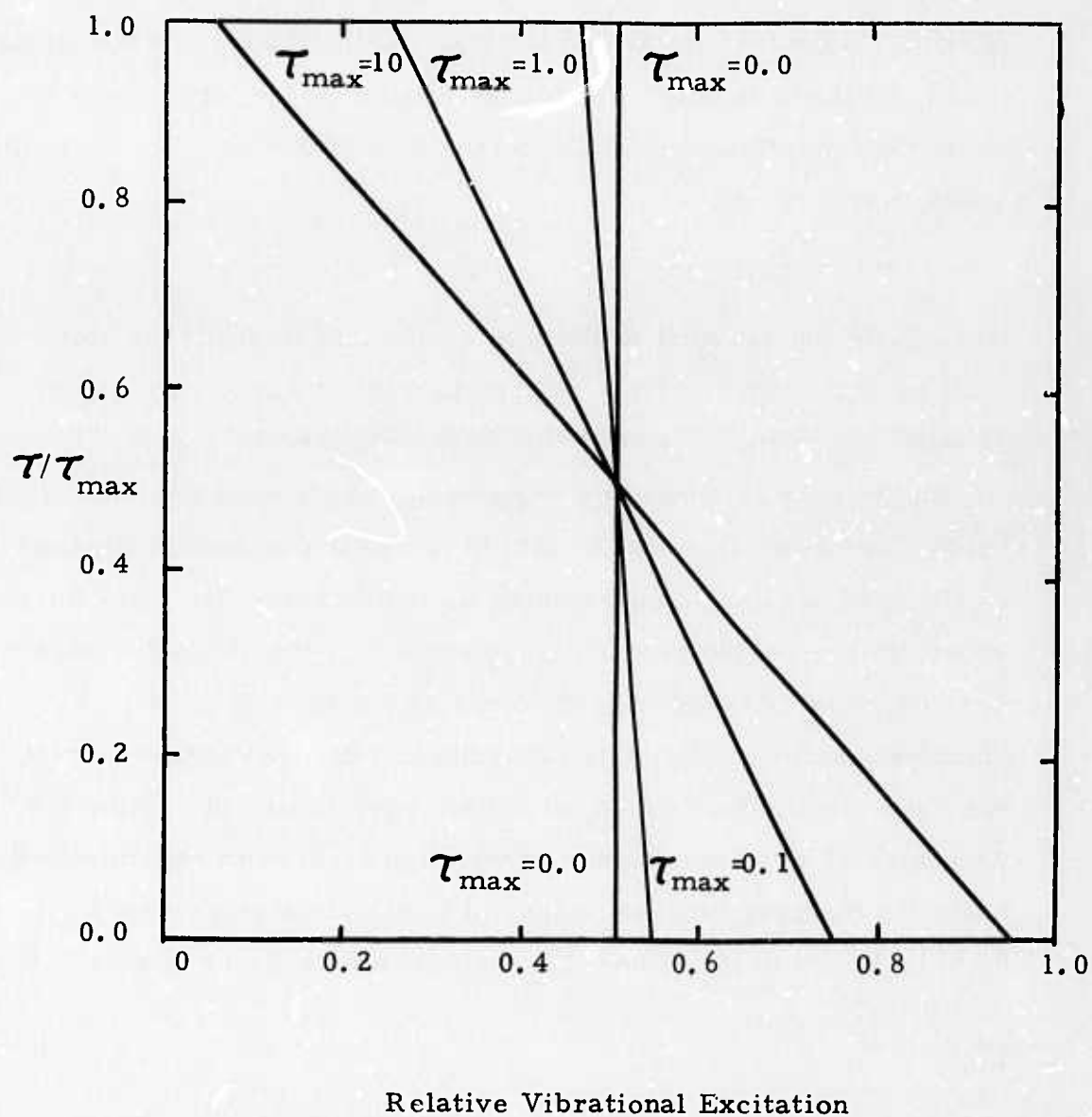


FIGURE II-2

effective excitation of the molecule at any point in the atmosphere is half that of a molecule at the (vibrational) temperature of the black body. As the total optical thickness increases, the excitation of the molecules near the black body increases, while that of molecules near the top of the atmosphere decreases. This occurs because as the optical thickness increases, molecules near the lower boundary absorb an increasing amount of radiation re-radiated from molecules above them. At the same time, less radiation penetrates to higher altitude. The physics of the problem require that if a second black body of the same temperature be placed at the top of the atmosphere, the population of radiators at all points would be uniformly that corresponding to the black body temperature. This symmetry and the linear character of the integral equation (2-1) results in the relation $J(\tau) + J(\tau_{\max} - \tau) = N_0$.

When a collimated beam of light is incident on the top of the atmosphere, another term must be added to the function $S(\tau)$ in equations (2-1) and (2-2) to account for this. If the flux is incident at a zenith angle with cosine μ and has an intensity in arbitrary units such as πF watts cm^{-2} normal to its direction, the term added to $S(\tau)$ has the form $FM_1[(\tau_{\max} - \tau)/\mu]$. In the gray case, $M_1(\tau)$ is simply $\exp(-\tau)$. The corresponding functions for individual spectral lines and bands will be described after a closer look at the interaction of electromagnetic radiation with a single molecule.

B. INTERACTION OF RADIATION WITH A SINGLE MOLECULE

When treating a problem in which the number of photons emitted or absorbed by an atom or molecule must be considered rather than total energy emitted, it is convenient to examine the physics of the

interaction of radiation with matter through use of the Einstein A and B coefficients. In treating a radiative problem such as the current study of high altitude infrared radiances which also involves transfer of energy between molecules through collisions, this approach is a necessity. In the following discussion, cgs units are used except where explicitly stated.

The Einstein A_{ul} coefficient is the rate at which an atom or molecule in an excited state spontaneously emits radiation. It has the units photons/sec-molecule. In an assemblage of molecules all in a state which can radiate, the average rate of radiation is given by the Einstein A_{ul} coefficient for the particular radiative transition from a state of higher energy (subscript u) to one of lower energy (subscript l).

In addition to spontaneous emission, two other processes occur. These are absorption, characterized by the Einstein coefficient for absorption B_{lu} , and induced emission, characterized by the Einstein coefficient for induced emission B_{ul} . In a black body radiation field with spectral density, ρ_{ν} , the probability that an atom or molecule absorbs a quantum of radiation in unit time is $B_{lu}\rho_{\nu}$. When radiation density is expressed in c. g. s. units, ergs-sec/cm³, the coefficient B_{lu} has units cm³/ergs-sec. Similarly, an atom or molecule in a radiation field with the above spectral density and in an excited state emits radiation at the rate $B_{ul}\rho_{\nu}$ in addition to that characterized by the coefficient A_{ul} . The Einstein coefficients are properties of an atom or molecule. If one coefficient is known, the others may be determined by the relations

$$A_{ul} = 8\pi h B_{ul} / \lambda^3 \quad (2-3)$$

and

$$g_l B_{lu} = g_u B_{ul} \quad (2-4)$$

Thus, it is possible to treat the problem knowing only the Einstein A_{ul} coefficient.

Experimental determinations of the interaction of infrared radiation with gases are usually made by measurements of light absorption. Experimental results may be expressed as integrated absorption from a continuum source,

$$S'_{lu} = N_l \frac{A_{ul} \lambda_{lu}^2}{8\pi} \frac{g_u}{g_l} \left[1 - \exp\left(-\frac{hc}{\lambda_{lu} kT}\right) \right] \quad (2-5)$$

or as line or band strengths

$$S_{lu} = S'_{lu}/p \quad (2-6)$$

where p is the pressure.

In the visible and ultraviolet regions of the spectrum, it is customary to use oscillator strengths to characterize the interaction of radiation and matter. In this case, the defining equation is

$$S'_{lu} = \frac{\pi e^2}{mc} N_l f_{lu} \left[1 - \exp\left(-\frac{hc}{\lambda_{lu} kT}\right) \right] \quad (2-7)$$

The results of theoretical computations of the interaction of matter with radiation are frequently expressed as dipole moments, μ_{ul} . These are related to the Einstein A coefficient by

$$A_{ul} = \frac{64\pi^4}{3h\lambda^3} \frac{g_l}{g_u} |\mu_{ul}|^2 \quad (2-8)$$

The rate at which a single atom or molecule absorbs and

reradiates light from a parallel beam from a continuum source at a wavelength λ_o corresponding to a resonance transition is (Mitchell and Zemansky, 1961):

$$G = \frac{\pi e^2}{mc^2} I_o f_o \lambda_o^2 \quad (\text{photons/sec})$$

$$= 8.852 \times 10^{-13} I_o f_o \lambda_o^2 \quad (\text{photons/sec}) \quad (2-9)$$

where I_o is the continuum source flux and f_o is the oscillator strength. If the incident flux is expressed in photons/cm²- μ m, and oscillator strength is replaced by the equivalent line or band strength S expressed as cm⁻²atm⁻¹, then

$$G = 3.72 \times 10^{-24} I_o S \lambda^2 \quad (2-10)$$

Implicit in this expression is the convenient relation between the Einstein A_{ul} coefficient and line or band strength with wavelength dimensions μ m

$$A_{ul} = 2.804 S (\text{cm}^{-2} \text{atm}^{-1}) / \lambda^2 (\mu\text{m}) \quad (2-11)$$

When the source is an extended black body surface with a spectral radiance N_λ , the G factor is obtained by integration over the solid angle subtended by the source. For radiation from a plane parallel surface of infinite extent,

$$G = 1.169 \times 10^{-23} N_\lambda S \lambda^2 \quad (2-12)$$

Another purely radiative mechanism of importance in upper atmosphere radiance computations is fluorescence. A striking example

occurs for the weak $10.4 \mu\text{m}$ CO_2 band. Absorption of solar radiation by CO_2 $4.3 \mu\text{m}$ band maintains the ν_3 vibrational mode at a vibrational temperature of about 290 K. During the day, this leads to an enhancement of emission in the $10.4 \mu\text{m}$ band by as much as two orders of magnitude when viewed along the earth's limb from outside the atmosphere.

Fluorescence occurs when the upper state of the resonance transition reradiates into other than the initial states. The relative probability of a radiative transition to a lower state, n from the upper state, u when there are k possible lower state is:

$$P_{un} = \frac{A_{un}}{\sum_{j=1}^k A_{uj}} \quad (2-13)$$

where the A_{uj} are the Einstein A coefficients for the spontaneous emission probabilities for a transition from the upper state to the j th lower state.

In the case of molecular resonance-fluorescent scattering at low temperature, only the lowest vibrational level ($v'' = 0$) in the ground electronic state is populated significantly. Absorption of a photon excites the molecule to a vibrational level, v' in the same or a higher electronic state. Radiation is possible from this state to the initial level ($v'' \neq 0$) or to other vibrational levels ($v'' = 0$) in the ground electronic state. The rate of resonance fluorescent scattering in a given electronic vibrational transition may be obtained by combining Equations (2-9) and (2-13) and introducing appropriate subscripts:

$$G_{v'v''} = 8.853 \times 10^{-17} I_{v'o} f_{v'o} \frac{2}{v'o} \frac{A_{v'v''}}{\sum_{v''} A_{v'v''}} \quad (2-14)$$

Here the subscript $v'v''$ refers to a transition from an upper state with vibrational level v' to a lower state with vibrational level v'' . The subscript $v'o$ refers to absorption of a photon by a molecule in the lowest vibrational level of the ground state, exciting the molecule to a vibrational level v' in the same or a higher electronic state.

C. RADIATIVE TRANSFER FUNCTIONS FOR LINES AND BANDS

In developing a realistic model of the interaction of radiation with matter, it is necessary to take into account the details of absorption. Line shape must be considered because it determines the amount of radiation escaping from an optically thick layer of gas. Thus, for large optical thickness (greater than a magnitude of about 10), the total emission from an isolated spectral line with Lorentz shape is proportional to the square root of the optical thickness, while that from a line with Doppler shape is proportional to the square root of the logarithm of the optical thickness. In addition, absorption of radiation emitted at one place in the gas by a molecule at another location cannot be computed without knowledge of the line shape.

At high altitudes, the profile of the spectral absorption curve of an individual line in a vibration-rotation band is predominantly due to velocity or Doppler broadening. Kuhn and London (1969), who investigated the heat budget of the atmosphere between 30 and 110 km, report that radiative transfer calculations require the use of the Voigt profile (including both collisional and Doppler broadening) at

altitudes between 20 and 70 km. Alternatively, the Doppler profile is adequate at higher altitudes where the Doppler shape is the largest contributor to line broadening. The original computational model therefore assumed a Doppler profile.

The discussion below assumes a Voigt profile for a single line, and it will be shown that for small optical thicknesses and low pressures, the difference between calculations with Doppler and Voigt profiles is small. Asymptotic values for large optical thicknesses are quite different, however.

The radiative transfer functions required to treat transfer of resonance radiation in a single line are well known for the Voigt profile and its two limiting cases, the Doppler and Lorentz profiles. Avrett and Hummer (1965) review the properties of four of these functions, giving series expansions for small values of optical thickness and asymptotic expressions for large values of the optical thickness. The notation used for these functions varies widely. That used here is adapted from that used by Ivanov and Shcherbakov (1965 a, b) in their tabulation of functions for the Doppler profile.

The best known of these functions is probably that relating to the equivalent width of a line in absorption or to the total radiation emitted in a line from a source in thermal equilibrium at a constant temperature, the integrated absorbance, defined as

$$L(a, \tau) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} (1 - e^{-\tau f(a, x)}) dx \quad (2-15)$$

Here $f(a, x)$ is used to denote the Voigt profile,

$$f(a, x) = \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{dt e^{-t^2}}{(t-x)^2 + a^2} \quad (2-16)$$

The parameter a is proportional to the ratio of the Lorentz half width at half maximum b_L and the Doppler half width at half maximum b_D ,

$$a = \frac{b_L}{b_D} (\ln 2)^{1/2} \quad (2-17)$$

The parameter x is proportional to the difference between the spectral frequency of the line center ν_0 and that at any other point in the line profile, ν

$$x = \frac{2(\nu - \nu_0)}{b_D} (\ln 2)^{1/2} \quad (2-18)$$

The quantity τ is the optical thickness at the center of a line with Doppler broadening alone,

$$\tau = \frac{2\pi e^2}{mc} \frac{Nfl}{b_D} (\ln 2)^{1/2} \quad (2-19)$$

where N is the number density of ground state molecules and l is the path length. The actual optical thickness at the center of a line with Voigt profile is the product of the τ of Equation (2-19) and $\exp(a^2)$ times the co-error function of the parameter a , $\text{erfc}(a)$. In general, Equation (2-15) must be evaluated numerically. For small values of τ , a series expansion may be obtained in the form

$$L(a, \tau) = - \sum_{n=1}^{\infty} \frac{(-\tau)^n}{n!} \Phi_n(a) \quad (2-20)$$

where

$$\Phi_n(a) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} [f(a, x)]^n dx \quad (2-21)$$

For all values of a , $\Phi_1(a)$ is one. When $\Phi_n(a)$ is divided by $\operatorname{erfc} a$, a smooth variation between $a = 0$ (Doppler profile) and $a = \infty$ (Lorentz profile) is obtained as shown in Figure (II-3) for small n . For large values of τ , asymptotic series are available, as given for example by van Trigt (1968).

$$L(0, \tau) \approx 2 \left(\frac{\ln \tau}{\pi} \right)^{1/2} \left[1 + \frac{.2886}{\ln \tau} + \dots \right] \quad (2-22a)$$

$$L(a \neq 0, \tau) \approx \frac{2(a \tau)^{1/2}}{(\pi)^{1/4}} \left[1 + \frac{\sqrt{\pi}}{8} \frac{3-2a^2}{a \tau} + \dots \right] \quad (2-22b)$$

Equation (2-10) gives the rate at which a single molecule absorbs radiation from a parallel beam. If the molecule is located within an optically thick medium, the rate of absorption of radiation is reduced by a factor which depends on the optical thickness,

$$M_1(a, \tau) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} f(a, x) e^{-\tau f(a, x)} dx \quad (2-23)$$

For small values of τ , a series expansion is

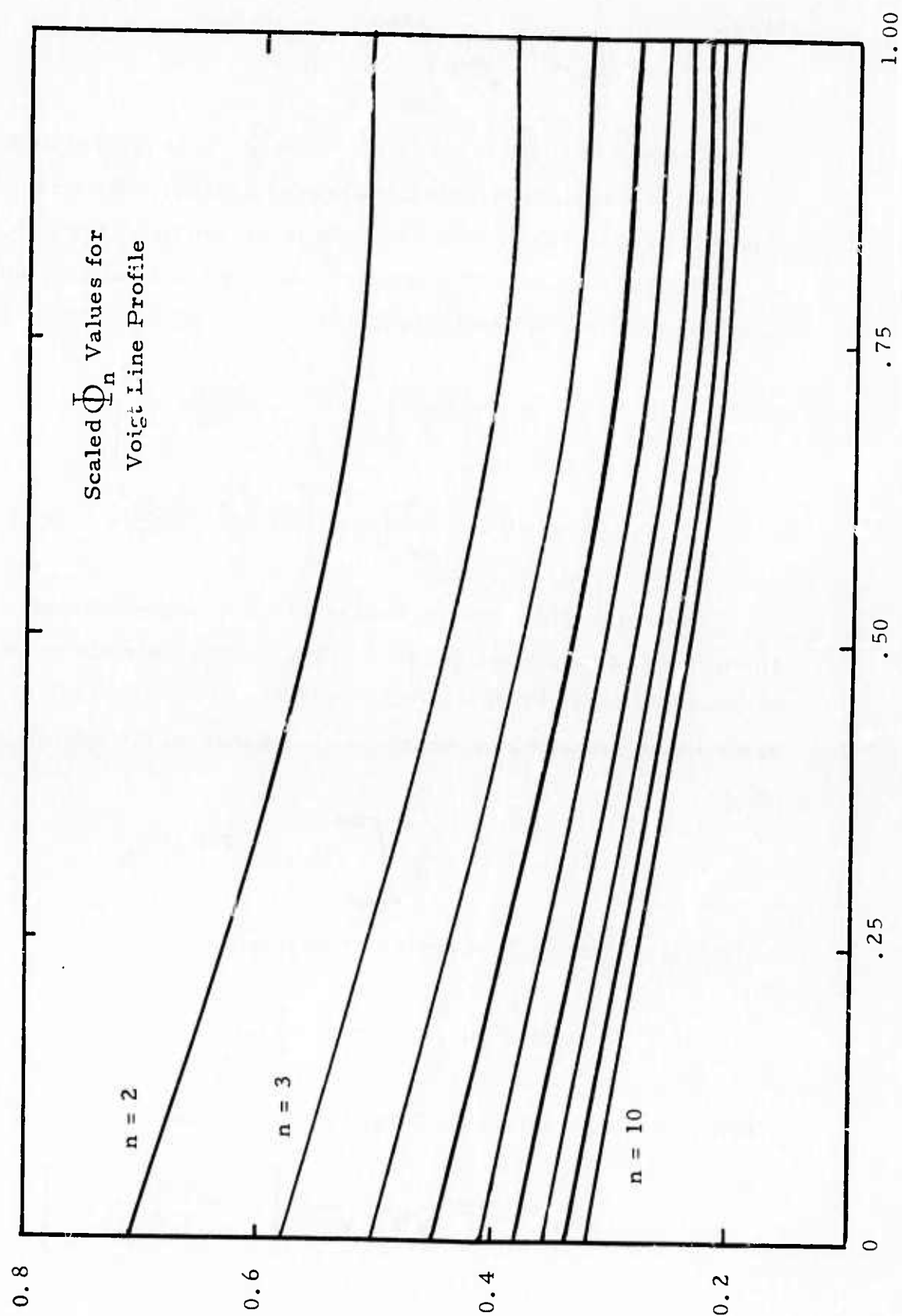
$$M_1(a, \tau) = \sum_{n=0}^{\infty} \frac{(-\tau)^n}{n!} \Phi_{n+1}(a) \quad (2-24)$$

Asymptotic expressions for large values of τ are

$$M_1(0, \tau) \approx \frac{1}{\sqrt{\pi \tau \ln \tau}} \left[1 - \frac{0.2886}{\ln \tau} + \dots \right] \quad (2-25a)$$

$a/(1+a)$

FIGURE II-3



$$M_1(a \neq 0, \tau) \approx \frac{1}{\pi^{1/4}} \sqrt{\frac{a}{\tau}} \left[1 - \frac{\sqrt{\pi}}{8} \frac{3-2a^2}{a\tau} + \dots \right] \quad (2-25b)$$

The function M_1 is the derivative with respect to τ of the function L . In addition to its use in modifying the G factor of Equation (2-10), it gives the probability of escape of a photon in a direction with optical thickness τ .

A third function is defined as

$$M_2(a, \tau) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} f(a, x)^2 e^{-\tau f(a, x)} dx \quad (2-26)$$

and has a series expansion

$$M_2(a, \tau) = \sum_{n=0}^{\infty} \frac{(-\tau)^n}{n!} \Phi_{n+2}(a) \quad (2-27)$$

This function is proportional to the rate at which a molecule absorbs radiation from another molecule at a optical distance τ . This function would be used as the kernel function K_1 in Equation (2-1) if one dimensional radiative transport were being treated. It is included here because of its use in generating the kernel function for a plane parallel geometry.

When the source of radiation is an infinitely extended plane black body, the function which is used to determine the rate at which a molecule absorbs radiation is given by

$$N_{12}(a, \tau) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} f(a, x) E_2[\tau f(a, x)] dx \quad (2-28a)$$

$$= \tau \int_{\tau}^{\infty} M_1(t) \frac{dt}{t^2} \quad (2-28b)$$

$$= \int_0^{\pi/2} M_1 \left(\frac{\tau}{\cos \theta} \right) \sin \theta d\theta \quad (2-28c)$$

The series expansion for this function is given by

$$N_{12}(a, \tau) = \Phi_1(a) + (\gamma \tau - \tau + \tau \ln \tau) \Phi_2(a) + \tau \Phi_L(a) - \sum_{n=2}^{\infty} \frac{(-\tau)^n}{(n-1)n!} \Phi_{n+1} \quad (2-29)$$

Here a new integral is defined,

$$\Phi_L(a) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} [f(a, x)]^2 \ln f(a, x) dx$$

and γ is the Euler-Mascheroni constant 0.5772... The asymptotic expansions

$$N_{12}(0, \tau) \approx \frac{1}{\sqrt{\pi} \tau \sqrt{\ln \tau}} \left(0.5 - \frac{0.2693}{\ln \tau} + \dots \right) \quad (2-30a)$$

$$N_{12}(a \neq 0, \tau) \approx \frac{1}{\pi^{1/4}} \left(\frac{a}{\tau} \right)^{1/2} \left(\frac{2}{3} + \dots \right) \quad (2-30b)$$

may be obtained from Equations (2-29b) and (2-25).

The kernel function for a plane parallel geometry is given by

$$N_{21}(a, \tau) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} [f(a, x)]^2 E_1[\tau f(a, x)] dx \quad (2-31a)$$

$$= \int_{\tau}^{\infty} M_2(t) \frac{dt}{t} \quad (2-31b)$$

$$= \int_0^{\pi/2} M_2 \frac{\tau}{\cos \theta} \frac{\sin \theta d\theta}{\cos \theta} \quad (2-31c)$$

The series expansion useful for small τ is

$$N_{21}(a, \tau) = -(\gamma + \ln \tau) \Phi_2 - \Phi_L - \sum_{n=1}^{\infty} \frac{(-\tau)^n}{n \cdot n!} \Phi_{n+2} \quad (2-32)$$

and the asymptotic expansions are

$$N_{21}(0, \tau) \approx \frac{1}{\sqrt{\pi} \tau^2 \sqrt{\ln \tau}} \left(0.5 - \frac{0.0193}{\ln \tau} + \dots \right) \quad (2-33a)$$

$$N_{21}(a \neq 0, \tau) \approx \frac{a^{1/2}}{\pi^{1/4} \tau^{3/2}} \left(\frac{1}{3} + \dots \right) \quad (2-33b)$$

The recurrence relation

$$N_{kn}(a, \tau) = \frac{1}{n-1} \left[M_k(a, \tau) - \tau N_{k+1, n-1}(a, \tau) \right] \quad (2-34)$$

carries over into the corresponding band functions and provides a partial check on numerical calculations.

In extending this treatment of radiative transfer to a vibration-rotation band, in addition to assuming that each line has the same Voigt profile shape, the following assumptions are made:

- (1) Rotational levels within a vibrational level remain in

equilibrium with the translational temperature.

This is valid up to at least 150 km according to Goody (1964).

- (2) There is complete redistribution of frequency within a single line following absorption of radiation.
- (3) There is complete redistribution of absorbed energy among all rotational levels.
- (4) Line strengths are used as if each line were at the band center, neglecting wavelength variation across a band.
- (5) There is no overlap of adjacent lines.
- (6) Temperature variations at different levels do not affect the radiative transfer.

Let g_J be the fraction of total band strength associated with a single line, so that

$$\sum_J g_J = 1 \quad (2-35)$$

and the sum over J may involve complete summation over rotational quantum number for two or more branches. The optical thickness at the center of a single line will be given by τg_J , where τ is the optical thickness that would result if the entire band strength were in a single line. Then the radiative transfer functions for a band may be defined as functions of radiative transfer functions for a single line. First,

$$L^b(a, \tau) = \sum_J L(a, \tau g_J) \quad (2-36)$$

where the superscript b refers to an entire band.

In order that the correct derivative relations

$$M_1^b(a, \tau) = \frac{d}{d\tau} L^b(a, \tau) \quad (2-37a)$$

$$M_2^b(a, \tau) = - \frac{d}{d\tau} M_1^b(a, \tau) \quad (2-37b)$$

and the integral relations of Equations (2-28b) and (2-31b) hold,

$$M_1^b(a, \tau) = \sum_J g_J M_1(a, \tau g_J) \quad (2-38a)$$

$$M_2^b(a, \tau) = \sum_J g_J^2 M_2(a, \tau g_J) \quad (2-38b)$$

$$N_{12}^b(a, \tau) = \sum_J g_J N_{12}(a, \tau g_J) \quad (2-38c)$$

$$N_{21}(a, \tau) = \sum_J g_J^2 N_{21}(a, \tau g_J) \quad (2-38d)$$

While these functions must be evaluated numerically, it is possible to perform this evaluation in two different ways for small values of τ . Making the definitions

$$G_n = \sum_J g_J \quad (2-39a)$$

$$G_L = \sum_J g_J^2 \ln g_J \quad (2-39b)$$

The following series expansions are obtained:

$$L^b(a, \tau) = - \sum_{n=1}^{\infty} \frac{(-\tau)^n}{n!} G_n \Phi_n(a) \quad (2-40a)$$

$$M_1^b(a, \tau) = \sum_{n=1}^{\infty} \frac{(-\tau)^n}{n!} G_{n+1} \Phi_{n+1}(a) \quad (2-40b)$$

$$M_2^b(a, \tau) = \sum_{n=0}^{\infty} \frac{(-\tau)^n}{n!} G_{n+2} \Phi_{n+2}(a) \quad (2-40c)$$

$$\begin{aligned} L_3^b(a, \tau) = & G_1 \Phi_1(a) \tau + \frac{1}{2} \left[\left(G_2 \ln \tau + G_L + \gamma - \frac{3}{2} \right) \Phi_2(a) \right. \\ & \left. + G_2 \Phi_L(a) \right] \tau^2 + \sum_{n=3}^{\infty} \frac{(-\tau)^n}{(n-2)n!} G_n \Phi_n(a) \end{aligned} \quad (2-40d)$$

$$N_{12}^b(a, \tau) = G_1 \Phi_1(a) + G_2 \Phi_2(a) \tau \ln \tau + \left[G_L \Phi_2(a) \right.$$

$$\left. + (\gamma - 1) G_2 \Phi_2(a) + G_L \Phi_L(a) \right] \tau -$$

$$- \sum_{n=2}^{\infty} \frac{(-\tau)^n}{(n-1)n!} G_{n+1} \Phi_{n+1}(a) \quad (2-40e)$$

$$\begin{aligned}
N_{21}(a, \tau) = & - \left[\gamma \Phi_2(a) + \Phi_L(a) \right] G_2 - G_2 \Phi_2(a) \ln \tau \\
& - G_L \Phi_2(a) - \sum_{n=1}^{\infty} \frac{(-\tau)^n}{n \cdot n!} G_{n+2} \Phi_{n+2}(a)
\end{aligned} \tag{2-40f}$$

For large values of the optical thickness parameter τ , there is a sharp distinction between the asymptotic expansions for Doppler line shape and Voigt line shape. When Doppler line shape is assumed, the asymptotic forms for the functions discussed above differ from those for a single line by a factor proportional to $(\ln \tau)^{1/2}$ in the case of bands for a linear molecule. The numerical results suggest that the asymptotic expansions for an asymmetric rotor are multiplied by an additional factor proportional to $\ln \tau$. In the case of a Voigt profile, there is no such change in the asymptotic form. The L functions retain their $\tau^{1/2}$ dependence, the M_1 and N_{12} functions retain the $\tau^{-1/2}$ dependence, and the M_2 and N_{21} functions retain the $\tau^{-3/2}$ dependence. The chief complication with the functions for Voigt profiles is that for intermediate values of τ the behavior is similar to that for a Doppler profile, while at some value of τ dependent on the parameter a , the functions begin to tend toward the asymptotic form. Similar behavior has been found by Malkmus (1967, 1968) for curves of growth for various random band models.

A strict derivation of the asymptotic expansions for the Doppler profile functions has not been obtained. In the high rotational temperature limit, the first term in the expansions for parallel and perpendicular bands of linear molecules appear to be

Parallel	Perpendicular	
$L^b(o, \tau) \sim \sqrt{\pi \epsilon} Q_R \ln \tau$	$\frac{3}{2} \sqrt{\pi \epsilon} Q_R \ln \tau$	(2-41a)

$M_1^b(o, \tau) \sim \sqrt{\pi \epsilon} Q_R / \tau$	$\frac{3}{2} \sqrt{\pi \epsilon} Q_R / \tau$	(2-41b)
--	--	---------

$M_2^b(o, \tau) \sim \sqrt{\pi \epsilon} Q_R / \tau^2$	$\frac{3}{2} \sqrt{\pi \epsilon} Q_R / \tau^2$	(2-41c)
--	--	---------

$L_3^b(o, \tau) \sim \frac{1}{2} \sqrt{\pi \epsilon} Q_R \ln \tau$	$\frac{3}{4} \sqrt{\pi \epsilon} Q_R \ln \tau$	(2-41d)
--	--	---------

$N_{12}^b(o, \tau) \sim \frac{1}{2} \sqrt{\pi \epsilon} Q_R / \tau$	$\frac{3}{4} \sqrt{\pi \epsilon} Q_R / \tau$	(2-41e)
---	--	---------

$N_{21}^b(o, \tau) \sim \frac{1}{2} \sqrt{\pi \epsilon} Q_R / \tau^2$	$\frac{3}{4} \sqrt{\pi \epsilon} Q_R / \tau^2$	(2-41f)
---	--	---------

Here Q_R is the rotational partition function and ϵ is hcB_v/kT , the dimensionless ratio of rotational quantum energy to kinetic temperature.

The first term in the asymptotic expansions for Voigt profile band functions is easily obtained, as is illustrated for the $L^b(a, \tau)$ function. At large optical paths, $L(a, \tau)$ for a single line is from Equation (2-21b) approximately $2\tau^{-1/4}(a\tau)^{1/2}$. Since the optical thickness at the center of a line in a band is simply $g_J \tau$, then

$$L^b(a, \tau) \sim 2\tau^{-1/4} a^{1/2} \sum_J (\tau g_J)^{1/2}$$

or, denoting $\sum_J g_J^{1/2}$ by $G_{1/2}$

$$L^b(a, \tau) \sim \frac{2}{\pi^{1/4}} (a\tau)^{1/2} G_{1/2} \quad (2-42a)$$

and

$$M_1^b(a, \tau) \sim \frac{(a/\tau)^{1/2}}{\pi^{1/4}} G_{1/2} \quad (2-42b)$$

$$M_2^b(a, \tau) \sim \frac{a^{1/2} G_{1/2}}{2\pi^{1/4} \tau^{3/2}} \quad (2-42c)$$

$$L_3^b(a, \tau) \sim \frac{4(a\tau)^{1/2}}{3\pi^{1/4}} G_{1/2} \quad (2-42d)$$

$$N_{12}^b(a, \tau) \sim \frac{2}{3\pi^{1/4}} \left(\frac{a}{\tau} \right)^{1/2} G_{1/2} \quad (2-42e)$$

$$N_{21}^b(a, \tau) \sim \frac{a^{1/2}}{3\pi^{1/4} \tau^{3/2}} G_{1/2} \quad (2-42f)$$

In order to simplify programming, a single set of functions is used for all parallel bands of linear molecules and a single set is used for perpendicular bands. These functions vary with the rotational temperature and in the program, in order to partially account for temperature variation, the parameter τ is not used, but rather a derived parameter τ_o , which is the optical thickness at the center of the strongest line in the band. This is either an R branch line for a parallel band or a Q branch line for a perpendicular band.

The effects of temperature variation will be illustrated by the

results of calculations for the $L^b(o, \tau)$ function for a perpendicular band of a linear molecule. The discussion assumes the Doppler profile because it is possible to obtain a series expansion for the high temperature limit in the variable τ_o . Use of double precision computation permits accurate calculation into the region where the logarithmic approximation to $L^b(o, \tau)$ becomes good.

The band used as an example is a "perpendicular" transition with upper state a $^1\pi$ level and lower state a $^1\Sigma$ level. It is assumed that the molecule is not symmetric and there are no nuclear spin effects. The relative strength of each line is the product of the exponential part of the Boltzmann factor of the rotational energy level of the lower state and the appropriated Hoehl-London transition probability or factor. For the J th rotational level, the Boltzmann factor is $\exp[-\epsilon J(J+1)]$ where $\epsilon = hcB_v/kT$ and h is Planck's constant, B_v is the rotational energy constant for the lower vibrational state, and k is Boltzmann's constant. The Hoehl-London factors for the P, Q, and R branches are

$$S_J^P = \frac{J-1}{2} \quad (2-43a)$$

$$S_J^Q = \frac{2J+1}{2} \quad (2-43b)$$

$$S_J^R = \frac{J+2}{2} \quad (2-43c)$$

and have been normalized so that the sum for a given value of J is $2J+1$.

The rotational partition function is the sum over all rotational levels of the product of the rotational degeneracy factor $2J + 1$ and the Boltzmann factor for each level. At high temperatures, an asymptotic approximation is available for the partition function.

$$Q_R = \sum_{J=0}^{\infty} (2J + 1) \exp [- \epsilon J(J + 1)] \quad (2-44a)$$

$$\approx \frac{1}{\epsilon} \left(1 + \frac{\epsilon}{3} + \frac{\epsilon^2}{15} + \frac{4\epsilon^3}{315} + \dots \right) \quad (2-44b)$$

The J value of the strongest line in the Q branch may be found by setting

$$\frac{d}{dJ} \frac{1}{2} (2J + 1) \exp [- \epsilon J(J + 1)] = 0 \quad (2-45)$$

and solving for J . The result is

$$J_{\max} = \frac{1}{2} \sqrt{\frac{2}{\epsilon}} - \frac{1}{2} \quad (2-46)$$

Adopting $Q_R \approx 1/\epsilon$, the fraction of band strength in the strongest line is $\sqrt{\epsilon/2} \exp(-1/2 + \epsilon/4)$ and the optical thickness at the center of this (fictitious) line is

$$\tau_o = \tau \sqrt{\epsilon/2} \exp (-1/2 + \epsilon/4) \quad (2-47)$$

using $k = \tau_o \sqrt{\epsilon/2} \exp (1/2 - \epsilon/4)$, the optical thickness at the center of any line in any branch is

$$\tau_J^P = k_o (J - 1) \exp [- \epsilon J(J + 1)] \quad (2-47a)$$

$$\tau_J^Q = k(2J+1) \exp[-\epsilon J(J+1)] \quad (2-47b)$$

$$\tau_J^R = k(J+2) \exp[-\epsilon J(J+1)] \quad (2-47c)$$

These expressions are then substituted in Equations (2-36) and (2-15) to obtain

$$L^b(o, \tau; \epsilon \rightarrow 0) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} \sum_{J; P, Q, R} \left(1 - e^{-k \tau_J^{(P, Q, R)} e^{-x^2}} \right) dx \quad (2-48)$$

where $f(o, x) = e^{-x^2}$ is used for the Doppler profile. The sum over J may be replaced by an integral over $z = J(J+1)$ and the summands $1 - \exp[-kf(z, x)]$ expanded in series and integrated over x and z . After simplification,

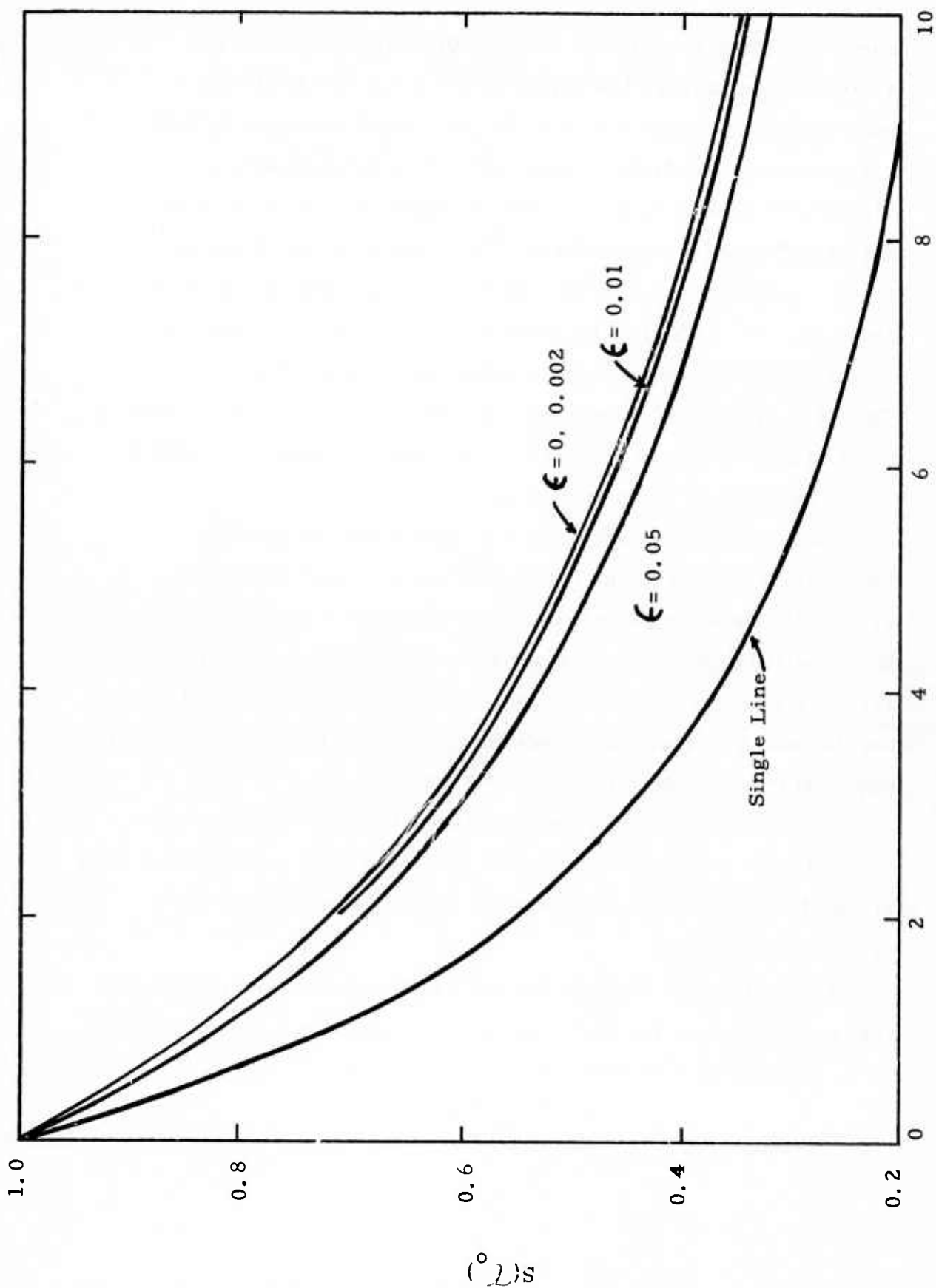
$$L^b(o, \tau; \epsilon \rightarrow 0) = \tau \sum_{n=1}^{\infty} \frac{(-\tau_o)^{n-1} e^{(n-1)/2}}{n; \sqrt{n}} (2^{n-1} + 1) (2n)^{-(n+1)/2} \Gamma\left(\frac{n+1}{2}\right) \quad (2-49)$$

Use of double precision arithmetic on the CDC 6600 permits evaluation of Equation (2-49) for values of τ_o up to about 50.

Define the function

$$S(\tau) = \frac{1}{\tau} L^b(o, \tau) \quad (2-50)$$

This function is plotted in Figure (II-4) for values of τ between zero and ten, using the series of Equation (2-49) for $\epsilon = 0$ and



Comparison of Values of $S(\tau_0)$ for Perpendicular Bands at Different Reduced Rotational Temperatures.

Note the more rapid decrease for a single line.

numerical integration for $\epsilon = 0.002, 0.01$ and 0.05 . On the scale of this drawing, the curves of $\epsilon = 0$ and $\epsilon = 0.002$ are indistinguishable, the values at $\tau = 10$ being 0.3501 and 0.3483 respectively. For larger values of τ , it is convenient to plot $\tau S(\tau)/\ln \tau$ versus $(\ln \tau)^{-1}$. This is shown in Figure (II-5) for values of τ between 10 and 50 for $\epsilon = 0$, and between 10 and 10^{100} for $\epsilon = 0.002, 0.01$ and 0.05 . At $\tau = 50$, the value for $\epsilon = 0$ is about one percent higher than that for $\epsilon = 0.002$. The value of $\epsilon = 0.05$ is about eight percent lower than that for $\epsilon = 0.002$. The finite values of ϵ used here correspond to rotational temperatures of about 280K , 56K , and 1.1K for carbon dioxide and 1400K , 280K , and 56K , for carbon monoxide.

The asymptotic behavior of the other radiative transfer functions is similar in the high temperature limit, taking into account the differences in the leading term of the expansion for large optical depth. In the upper atmosphere, the region in which radiative transfer is the most significant factor affecting vibrational populations is at such an altitude that the Doppler shape is the main contributor to the effects of radiative transfer.

The next step is to fit these radiative transfer functions into the context of obtaining a solution to Equation (2-1) and the extensions of Equation (2-1) when the effects of collisional excitation and de-excitation are added.

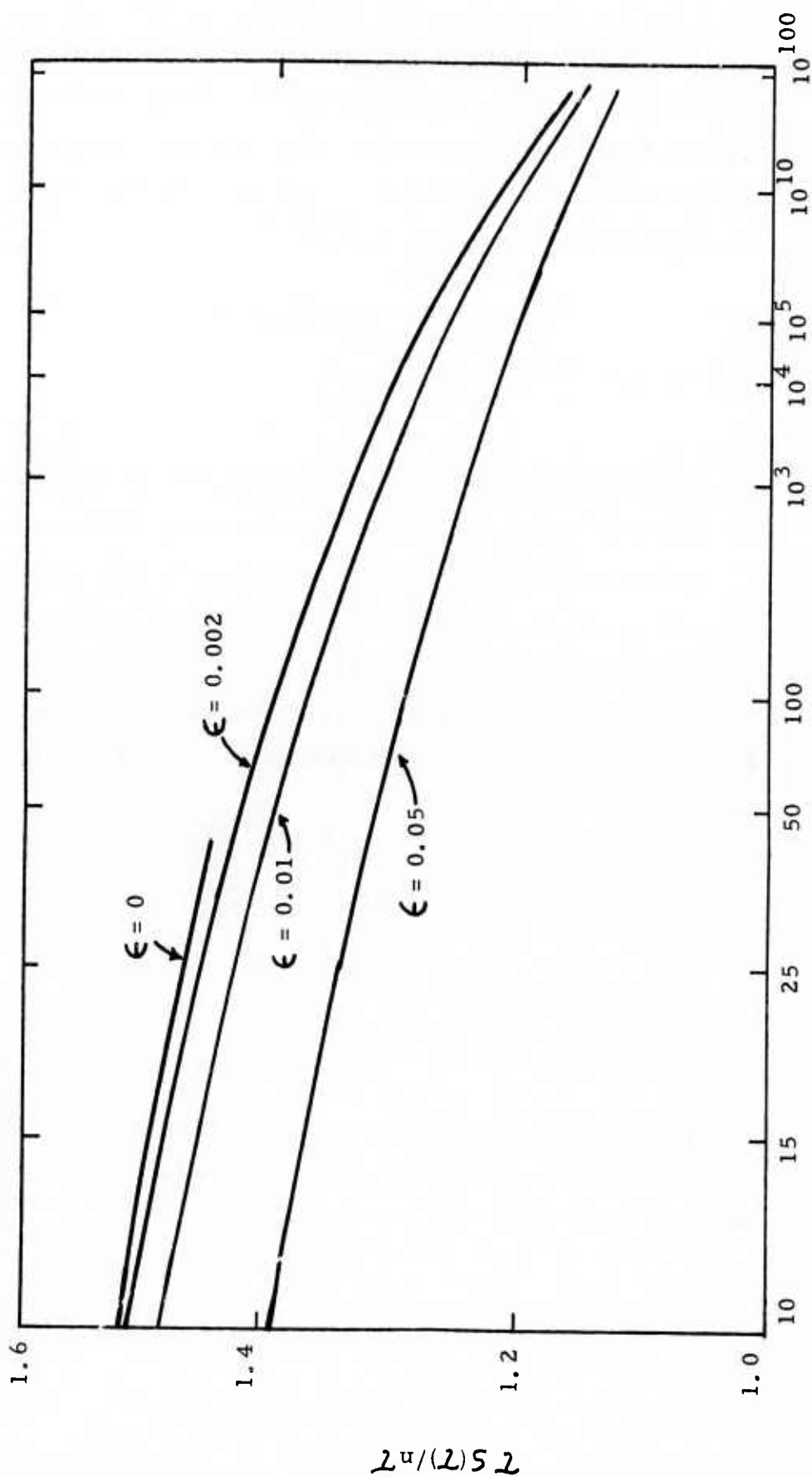
A definite lower limit to the source function at the far boundary may be obtained by assuming the source function to be linear in τ . In the gray case, this leads to

$$J(\tau) = \frac{1 - 2\epsilon_3(\tau_0)}{2(1 + \tau_0 - e^{-\tau_0})} \quad (2-51)$$

FIGURE II-5

Comparison of Values of $\tau_o S(\tau_o) / \ln \tau_o$ for Perpendicular Bands at
Different Reduced Rotational Temperatures and Large Values of the

Optical Thickness τ



τ

$\tau_o S(\tau_o) / \ln \tau_o$

where τ_o again refers to the total optical path length through a finite plane layer. This expression is never in error by more than 13.4%, when compared with King's (1956) exact solution. Making the same approximation for line or band radiative transport functions gives the result

$$J(\tau_o) = \frac{2L_3(\tau_o)}{\tau_o + L(\tau_o)} \quad (2-52)$$

This becomes increasingly inaccurate as the optical path through the layer increases, because of the long range effects of line shape.

Ivanov (1972) has obtained an asymptotic solution to two radiative transfer problems involving line radiation with arbitrary line shape. The first is that of a plane layer of finite optical thickness τ_o in which one boundary layer is in radiative equilibrium and is the sole source of radiative flux to the medium. The corresponding integral equation is

$$\begin{aligned} \Phi(\tau, \tau_o) = & \frac{\lambda}{2} \int_0^{\tau_o} \Phi(t, \tau_o) N_{21}(|t - \tau|) dt \\ & + \frac{\lambda}{2} N_{21}(\tau) \end{aligned} \quad (2-53)$$

The parameter λ allows for loss of radiation by "true" absorption or collisional de-excitation. The asymptotic solution to this equation when τ_o is very large is

$$\Phi^a(\tau, \tau_o) = \frac{\frac{\lambda}{2} N_{21}(\tau)}{[1 - \lambda + \lambda N_{12}(\tau)]^{3/2}} \left(\frac{1 - \lambda + \lambda N_{12}(\tau_o)}{1 - \lambda + \lambda N_{12}(\tau_o - \tau)} \right) \quad (2-54)$$

The second problem is that of a plane layer with a constant excitation mechanism and no external source of radiation. The integral equation is

$$S(\tau) = \frac{\lambda}{2} \int_0^{\tau_o} N_{21}(\tau - t) S(t) dt + 1 \quad (2-55)$$

and the asymptotic solution is

$$S^a(\tau) = [1 - \lambda + \lambda N_{12}(\tau)]^{-1/2} [1 - \lambda + \lambda N_{12}(\tau_o - \tau)]^{-1/2} \quad (2-56)$$

This last result may then be used to provide an asymptotic solution to the earthshine problem with no collisions, in which case λ is equal to one. A lower limit to the excitation from below is $\frac{1}{2} N_{12}(\tau_o)$. From symmetry,

$$\Phi(\tau_o/2, \tau_o) = \frac{1}{2} \quad (2-57a)$$

$$\Phi(\tau, \tau_o) = 1 - \Phi(\tau_o - \tau, \tau_o) \quad (2-57b)$$

A lower (in the asymptotic case of large τ_o) limit to the source function for τ greater than $\tau_o/2$ is then

$$\Phi^a(\tau, \tau_o) = \frac{1}{2} \frac{N_{12}(\tau_o)}{[N_{12}(\tau) N_{12}(\tau_o - \tau)]}, \tau \geq \tau_o/2 \quad (2-58)$$

This gives low values in the interior, and a bridging formula which gives a good initial solution which can be refined by iteration is

$$\Phi^a(\tau, \tau_o) = \frac{1}{2} [N_{12}(\tau)/N_{12}(\tau_o - \tau)]^{1/2}, \tau \geq \tau_o/2 \quad (2-59)$$

This can be used with Equation (2-57b) to cover the entire range of τ from zero to τ_o .

In practice, rather than formally integrate a modified Equation (2-1) including a τ dependent λ to account for collisional de-excitation, and an additional source term to account for collisional excitation, the computer program sets an initial vibrational population at each altitude and computes the total radiative excitation at each level which results from the sum of radiation from the earth and lower atmosphere, the sun and other levels in the atmosphere.

The band functions are used to determine the effects of absorption between a molecule at a given altitude and the various sources of radiation affecting a given band in the following way. The vertical optical paths to the lower boundary and to each level in the atmosphere are computed and, for daytime conditions, the optical path to the assumed top of the atmosphere in the direction of the sun using the secant of the solar zenith angle as a multiple. The effective radiation from the lower boundary is determined by multiplying the surface radiancy by the appropriate N_{12}^b function. The effective radiation from the sun is determined by use of the proper M_1^b function. The effective radiation from the other levels of the atmosphere may be obtained by integrating the product of emission at each level and the band function N_{21}^b . This is no

longer done directly, however, as it was discovered that the earlier integration subroutine gave incorrect results. Instead, the assumption is now made that the relative vibrational population between two points varies linearly with optical thickness. Then the integral relations between the band functions are used in the form

$$\begin{aligned} \int_{\tau_1}^{\tau_2} J(t) N_{21}^b(a, t) dt &= \int_{\tau_1}^{\tau_2} (A + Bt) N_{21}^b(a, t) dt \\ &= J(\tau_1) N_{12}^b(a, \tau_1) - J(\tau_2) N_{12}^b(A, \tau_2) \\ &\quad + \frac{J(\tau_2) - J(\tau_1)}{\tau_2 - \tau_1} \left[L_3^b(A, \tau_L) - L_3^b(a, \tau_1) \right] \quad (2-60) \end{aligned}$$

Vibrational populations are determined by balancing collisional and radiative excitation and de-excitation rates. Total band intensities at an observation point inside or outside the atmosphere are computed by determining the optical path from each level to the observation point and integrating the product of local emission rate and the band function $M_1^b(a, \tau)$. The spectral distribution of radiation is determined by finding a mean effective temperature and line of sight column density for the radiating molecules, computing intensity for each line in the band with the line function $L(a, \tau)$, summing the line emission rates and scaling each line emission rate so that the total band intensity is obtained.

The above analysis has been presented for the general Voigt profile. Actual use of the radiative transfer functions in the programs has been restricted to the Doppler profile. This restriction is adequate for the water vapor and ozone bands which in the concentrations used in the program have a maximum vertical optical thickness at line center less than 3. For limb viewing of carbon dioxide bands the Voigt profile should be used. Efforts to find a general way of setting up the radiative transfer functions to use a Voigt profile that varies with altitude have not been successful. Exploratory calculations show that the computed radiance values for strongest bands at a tangent height of 60 kilometers may be in error by 20 -- 50 %. In view of the uncertainties in chemical abundances, this error is not felt to be serious.

The same radiative transfer functions have been used for the non-linear molecules as were used for the linear molecules. The match between radiative transfer functions has been made by determining a single "effective" rotational constant for the non-linear tri-atomic molecules. This was done by computing actual radiative transfer functions for a limited range of optical thicknesses adequate to cover that needed in the model. The computed functions were compared with those for the linear molecules and the effective rotational constant needed to produce an approximate match at optical thickness at line center of about 2 was used.

SECTION III

ATMOSPHERIC COMPOSITION

There have been relatively few measurements of the variation with altitude of infrared emitting species at altitudes above 40 km, the limit of direct sampling by balloons. While ozone measurements by different workers agree reasonably well with each other and with theoretical computations at altitudes up to 100 km, and nitric oxide profiles appear reasonably well known between about 80 and 150 km at middle latitudes, corresponding data are lacking for other species which are important. There is in some cases indirect data available which when combined with computational models can yield limits to concentrations. Thus, Anderson (1971 a) has been able to put an upper limit on total hydroxyl radical abundance above 60 km from measurement of resonance fluorescence and with this result computes possible water vapor profiles between 50 and 100 km using a photochemical model that includes vertical transport by eddy diffusion. In a later paper, Anderson (1971 b) gives a measured altitude profile for hydroxyl with error limits ± 120 per cent.

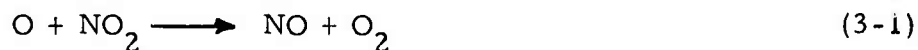
At present, then, estimates of chemical abundances of minor species required to predict infrared radiation require the use of photochemical computations. Even with the inclusion of best estimates of the effects of such transport processes as eddy mixing, these computations must be used with caution, even when they appear to agree with the limited concentration determinations that are available. Wofsy and McElroy (1973) give a discussion of methane concentrations in the stratosphere which illustrates the interplay of experiment and

modelling studies, showing how estimates of eddy mixing coefficients may be obtained.

A knowledge of the rates of the appropriate chemical reactions is necessary in order to estimate the abundance of trace constituents at high altitudes in the earth's atmosphere. A set of reaction rates, with estimates of probable error in the rates was listed in the final report on the previous research (Degges, 1972). This list was necessarily incomplete and several of the rates quoted were only estimates. Several reactions have been measured only at room temperature and others only at flame temperatures. In the latter case, only upper or lower bounds may be known.

Since that report was completed, a series of evaluations of chemical reaction rate coefficients has been published by workers at the National Bureau of Standards as a part of the Department of Transportation Climatic Impact Assessment Program. The most recent of these compilations, edited by Garvin and Hampson (1974) provides a thorough summary and evaluation of the accuracy of rate coefficients for neutral chemical relations and photochemistry, vibrational energy transfer processes, high temperature air reactions, and ion-molecule reactions. These reports are the main source of data used in updating the chemistry program.

Among the most important new measurements which have been made are those of Davis, Herron and Huie at temperatures between 200 and 350 K for the reactions



and



Reaction (3-1) is found to be temperature independent with a rate constant $9.1 \times 10^{-12} \text{ cm}^3/\text{molec-sec}$ in contrast to the $\exp(-300/T)$ temperature dependence of the analysis of Baulch, et al (1970) which we have used previously. Reaction (3-2) is found to have a temperature dependence of $\exp(500/T)$ rather than the $\exp(1060/T)$ given by Johnston (1968) and is slower at low temperatures than previously believed. This implies slower ozone formation and slightly greater atomic oxygen concentrations at high altitudes.

Many reaction rates remain poorly determined, and the compilation of Garvin and Hampson points these out clearly. One such reaction is



where measurements of the rate range between 10^{-11} and $2 \times 10^{-12} \text{ cm}^3 \text{ molecules}^{-1} \text{ s}^{-1}$. They suggest that model calculations should include the extreme ranges.

Water vapor abundances are not well known, even in the stratosphere. Balloon measurements are limited to altitudes below 40 km and are subject to considerable uncertainty as to the amount of water vapor carried to high altitude by the balloon. Direct measurements put lower and upper limits of the volume mixing ratio at two and ten parts per million in the upper stratosphere. A recent optical measurement from a balloon has been made by Goldman, et al (1973) who observed thermal emission from the rotational spectrum near 25 micrometers. Near and below 30 km, the volume mixing ratio is nearly three parts per million. In the region between 30 and 36 km, above the peak altitude reached by the balloon, the mixing ratio appears to be two or three times as large. Scholz, et al (1970)

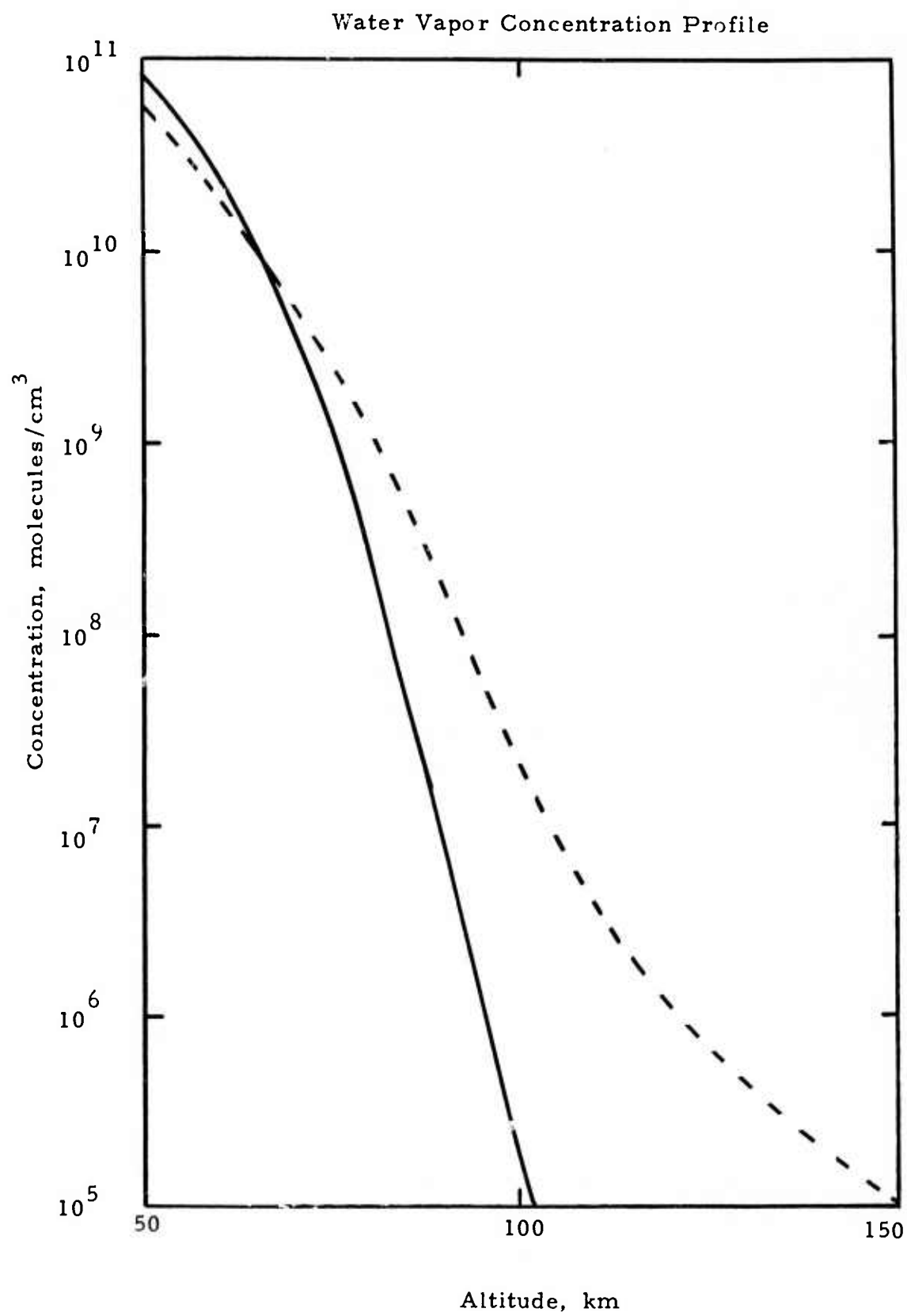
obtained comparable results in a direct sampling from a rocket near 50 km. Hunten and Stroebel (1974) have reviewed measurements and computations. They present a model which assumes a mixing ratio of four parts per million at 30 km. This includes the water producer by oxidation of methane in the stratosphere. Figure III-1 shows the results of their computation (solid line) and the water vapor profile used by Degges (1972), (dashed line). Hunten and Strobel (1974) show that their results are relatively insensitive to variations in the eddy mixing processes. Except for very large changes in the mixing ratio at the 30 km level, water vapor concentrations at all altitudes will vary directly with the low altitude mixing ratio. They find that better agreement can be obtained with Anderson's (1971 a, b) measurements if half as much water is assumed to be present in the atmosphere.

Figure III-2 shows a typical nitric oxide concentration curve, based on mid-latitude measurements.

While ozone abundances below about 50 km must take into account lateral transport as well as vertical transport by eddy mixing and molecular diffusion, photochemical models are adequate above that altitude, and agree with observations obtained by measuring absorption of solar and stellar ultraviolet radiation and those deduced from measurements of the molecular oxygen $1.27\mu\text{m}$ infrared atmospheric band. The exact profile depends on assumed eddy diffusion coefficients, however, principally through atomic hydrogen and oxygen concentration. O_3 abundances used here are shown in Figure III-3.

Carbon dioxide has a lifetime of about 10 days at the top of the atmosphere, where it is dissociated by solar radiation. It is well shielded by molecular oxygen below about 120 km, however, and should remain well mixed below 100 km. The only good measurement

FIGURE III-1



Nitric Oxide Concentration Profiles

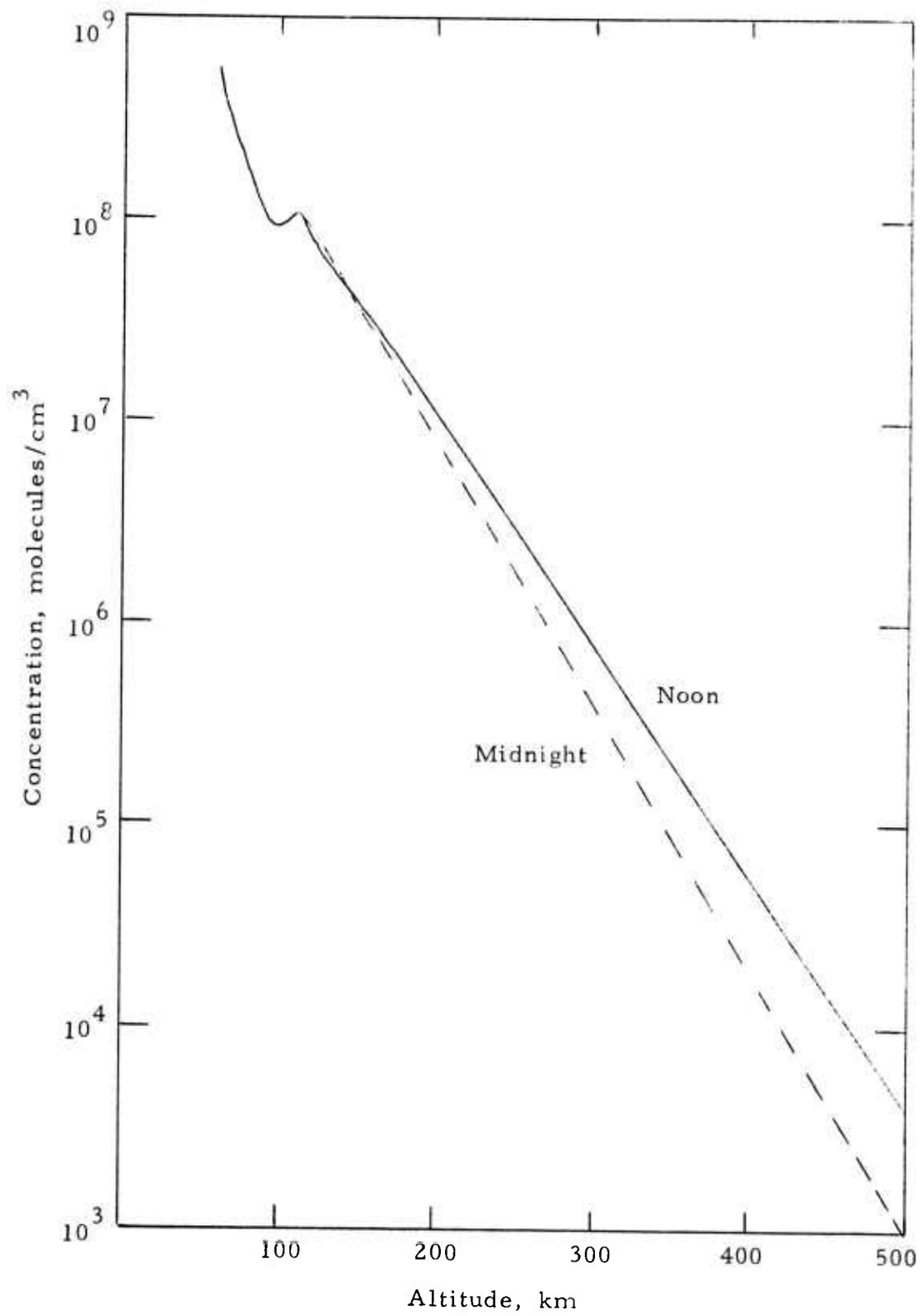


FIGURE III-2

Ozone Concentration Profiles

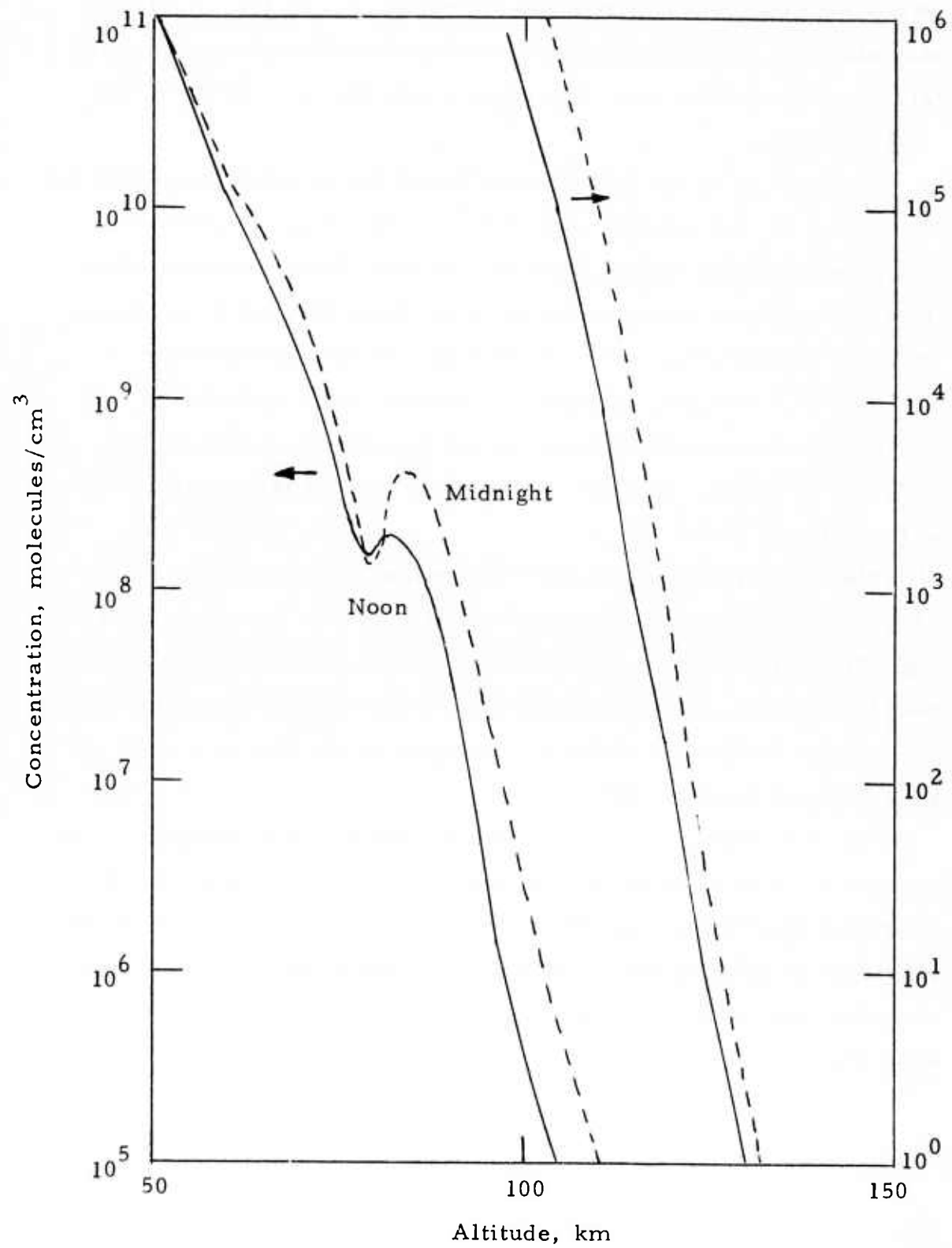


FIGURE III-3

above 100 km remains that of Offerman and von Zahn (1971), who find that between 120 and 140 km the mixing ratio is not more than 50 per cent less than the tropospheric value. Above 140 km, molecular diffusion is rapid enough compared to photodissociation to maintain diffusive equilibrium. Figure III-4 is a typical estimate of CO_2 concentrations.

Recent work by Liu and Donahue (1974) has resulted in a model for H_2O , CH_4 , H_2 and odd hydrogen that properly relates the measured mixing ratios in the stratosphere to escape of atomic hydrogen from the atmosphere by the mechanisms of the Jeans thermal flux, charge exchange and the polar wind. Their water vapor concentrations derived for a 1000 K exospheric temperature differ from that of Figure III-1 by less than a factor of two for altitudes below 100 km. At higher altitudes, their values become somewhat larger than those of the drawing.

The implication is that, since the chemistry program used here does not include the proper boundary conditions for hydrogen escape at high altitudes, long time calculations for hydrogen containing species may be in error. Future modifications to the chemistry program should include a provision for adding the hydrogen escape flux as part of the high altitude boundary conditions.

The chemistry program is described and listed in Appendix A, in almost the same form as used by Degges (1972). In addition to modification of the boundary conditions, it may be possible to improve the efficiency of the integration method. The remainder of this section describes the results of an investigation of a modification of the basic algorithm.

Carbon Dioxide Concentration Profile

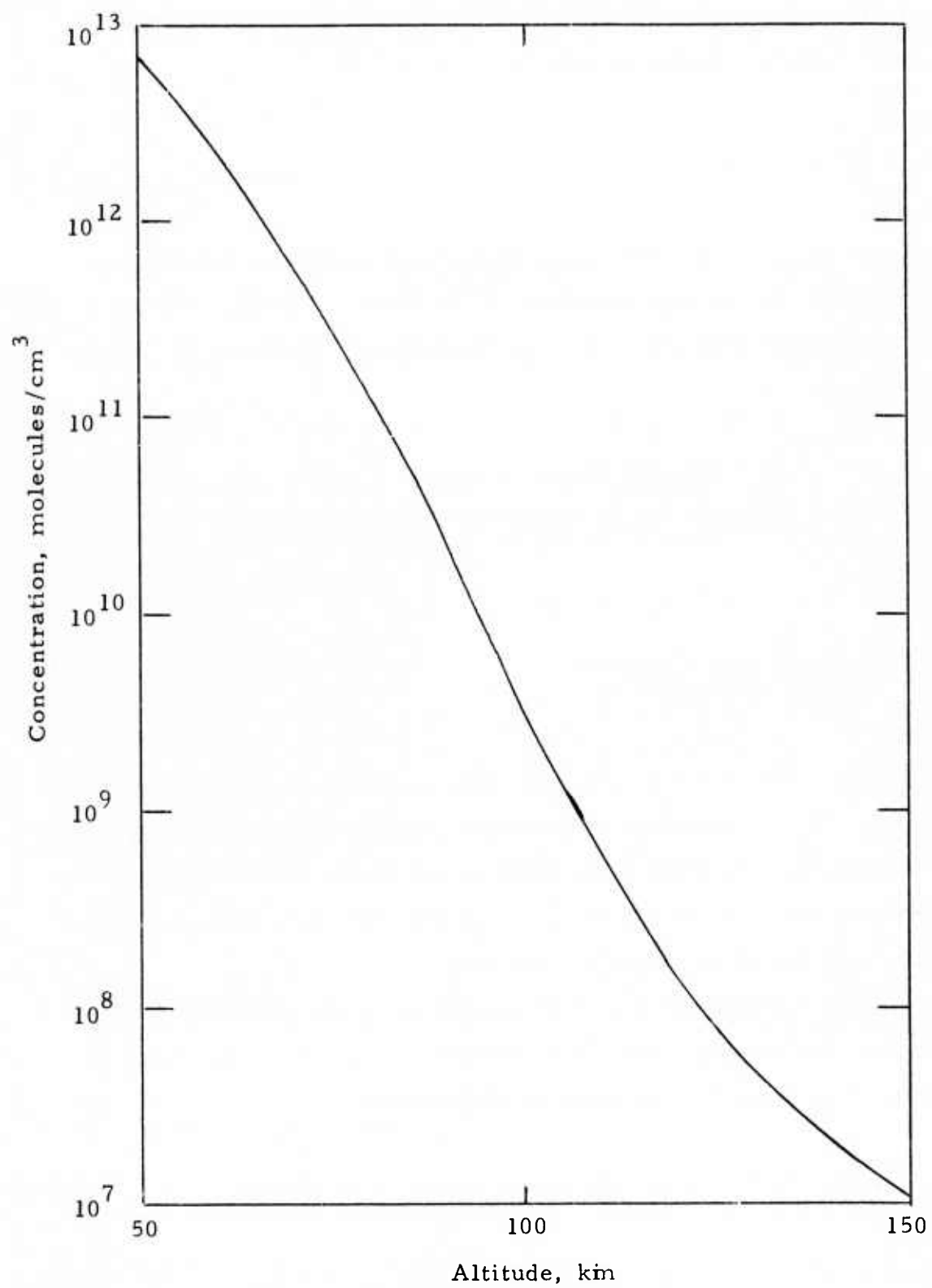


FIGURE III-4

The numerical method used to integrate the chemical rate equations in the chemistry program assumes that the rate equation for a single molecular species may be written

$$\frac{dx}{dt} = q - \beta x - \alpha x^2 \quad (3-4)$$

where q , β , and α are time dependent functions of the rate coefficients and the concentrations of the other molecular species in the system. The analytical solution of equation (3-4) for q , β , and α constant,

$$x(t) = \frac{[(\beta + \sigma)\exp(-\sigma t) + (\sigma - \beta)]x_0 + 2q[1 - \exp(-\sigma t)]}{(2\alpha x_0 + \beta)[1 - \exp(-\sigma t)] + \sigma[1 + \exp(-\sigma t)]} \quad (3-5)$$

where

$$\sigma = (\beta^2 + 4\alpha q)^{1/2}$$

is applied within the framework of the second order improved tangent Runge - Kutta method as described by Degges (1972). This algorithm is stable for any value of the time t and avoids the necessity of assumptions such as that some reactants with extremely short time constants are in chemical equilibrium.

When the product σt is large and any of the quantities q , β , and α are changing with time, however, true time dependence is lost. For large σt , equation (3-5) becomes

$$x(t) = \frac{\sigma - \beta}{2\alpha} = \frac{2q}{\sigma + \beta}, \quad \sigma t \text{ large} \quad (3-6)$$

and the value computed for the time t actually corresponds to time $t/2$ when Equation (3-5) is embedded in any second order Runge - Kutta method. In effect, the basic step is only first order for molecular species for which σt is large. The extrapolation algorithm does converge to a value for the concentrations of such components, but the process may require more steps than if the basic step were truly second order, as it is for small values of σt , or when q , β , and are constant.

Modifications of the algorithm has been attempted as follows. Consider the differential equation

$$\frac{dx}{dt} = q - \beta x \quad (3-7)$$

which is Equation (3-4) with the x^2 term absent. The formal solution for q and β constant is

$$x(t) = x \exp(-\beta t) + (q/\beta)[1 - \exp(-\beta t)] \quad (3-8)$$

If q and β are functions of time,

$$q = q_0 + q_1 t + q_2 t^2 + \dots \quad (3-9a)$$

$$\beta = \beta_0 + \beta_1 t + \beta_2 t^2 + \dots \quad (3-9b)$$

The improved tangent method applied over an interval h results in:

$$x(h/2) = x_0 + (h/2)(q_0 - \beta_0 x_0) \quad (3-10)$$

$$\frac{dx}{dt} = q_0 + (h/2)q_1 + (h/2)q_2 + \dots$$

$$- [\beta_0 + (h/2)\beta_1 + (h/2)^2\beta_2 + \dots][x_0 + (h/2)(q_0 + \beta_0 x_0)] \quad (3-11)$$

and

$$x(h) = x_0 + h \left. \frac{dx}{dt} \right|_{h/2}$$

$$= x_0 + hq_0 + (h^2/2)q_1 - h\beta_0 x_0 - (h^2/2)\beta_1 x_0$$

$$- (h^2/2)\beta_0^2 x_0 + \text{terms in } h^3, h^4, \dots \quad (3-12)$$

which is correct through in terms in h^2 .

When Equation (3-8) is embedded in the improved tangent method, the result is:

$$x(h/2) = x_0 \exp(-\beta_0 t) + (q_0/\beta_0)[1 - \exp(-\beta_0 t)] \quad (3-13)$$

$$\left. \frac{dx}{dt} \right|_{h/2} = q_0 + (h/2)q_1 + (h/2)^2 q_2 + \dots \quad (3-14)$$

$$- [\beta_0 + (h/2)\beta_1 + (h/2)^2\beta_2 + \dots] x(h/2)$$

and

$$x(h) = x_0 \exp[-h\beta_0 - (h/2)\beta_1 - \dots] \quad (3-15)$$

$$+ \frac{q_0 + (h/2)q_1 + \dots}{\beta_0 + (h/2)\beta_1 + \dots} [1 - \exp[-h\beta_0 - (h/2)\beta_1 - \dots]]$$

A series expansion of Equation (3-15) is identical to Equation (3-12) through terms in second order. The higher order terms are different, but the method is still second order. For large βh , however, Equation (3-15) becomes

$$x(h) \simeq \frac{q_0 + (h/2)q_1 + (h/2)^2 q_2 + \dots}{\beta_0 + (h/2)\beta_1 + (h/2)^2 \beta_2 + \dots} \quad (3-16)$$

and not the correct result

$$x(h) \simeq \frac{q_0 + hq_1 + h^2 q_2 + \dots}{\beta_0 + h\beta_1 + h^2 \beta_2 + \dots} \quad (3-17)$$

When βh is large, the algorithm may be altered as follows to retain second order accuracy and obtain a better approximation to the endpoint value. Let:

$$x = q/\beta + \phi$$

Then

$$\begin{aligned} \frac{d\phi}{dt} &= -\frac{d}{dt} \frac{q}{\beta} - \beta\phi \\ &= \phi - \beta\phi \end{aligned} \quad (3-18)$$

and

$$\phi = \phi_0 \exp(-\beta t) + (\phi/\beta)[1 - \exp(-\beta t)] \quad (3-19)$$

further, let

$$\phi = \phi/\beta + \Psi$$

then

$$\begin{aligned} \frac{d\Psi}{dt} &= - \frac{d}{dt} \left(\frac{\phi}{\beta} \right) - \beta \Psi \\ &= R - \beta \Psi \end{aligned} \quad (3-20)$$

and

$$\Psi = \Psi_0 \exp(-\beta t) + (R/\beta)[1 - \exp(-\beta t)] \quad (3-21)$$

Only terms in q_0 , q_1 , β_0 , and β_1 enter into the second order terms in the solution of Equation (3-7) given in Equation (3-12). If q and β are assumed linear in the interval of integration h , $q_0 = q(t=0)$, $\beta_0 = \beta(t=0)$, $q_1 = 2[q(h/2) - q_0]/h$, $\beta_1 = 2[(h/2) - \beta_0]/h$, and if $\phi_0 = x_0 - q_0/\beta_0$,

$$x(h/2) = q_0/\beta_0 + \phi_0 \exp(-\beta_0 h/2) \quad (3-22)$$

Then if $\Psi_0 = \phi_0 - \frac{\beta_1 q(h/2) - q_1 \beta_0(h/2)}{\beta^2(h/2)}$ and the term R is

neglected, $\Psi(h) = \Psi_0 \exp[-h\beta(h/2)]$ and the resulting expression

$$\begin{aligned}
 x(h) = & \frac{q_0 + h q_1}{\beta_0 + h \beta_1} + \frac{\beta_1 q_0 - \beta_0 q_1}{(\beta_0 + h \beta_1/2)^3} [1 - \exp(-h \beta_0 - h^2 \beta_1/2)] \\
 & + (x_0 - \frac{q_0}{\beta_0}) \exp(-h \beta_0 - h^2 \beta_1/2)
 \end{aligned} \tag{3-23}$$

when expanded in series, agrees through terms in h^2 with Equations (3-12).

The same analysis may be applied to Equation (3-4). In this case the appropriate substitution is;

$$\begin{aligned}
 x &= \frac{2q}{\sigma + b} + \phi \quad \text{and} \\
 \phi &= -\frac{d}{dt} \frac{2\sigma}{\sigma + b} - \sigma \phi - \alpha \phi^2 \\
 &= \phi - \sigma \phi - \alpha \phi^2
 \end{aligned} \tag{3-24}$$

setting

$$\Delta^2 = \sigma^2 + 4\alpha\phi, \text{ make the further substitution}$$

$$\phi = \Psi + \frac{2\phi}{\Delta + \sigma}$$

to obtain

$$\begin{aligned}
 \Psi' &= -\frac{d}{dt} \left(\frac{2\phi}{\Delta + \beta} \right) - \Delta \Psi - \alpha \Psi^2 \\
 &= R - \Delta \Psi - \alpha \Psi^2
 \end{aligned} \tag{3-25}$$

Again neglecting the R term in Equation (3-25), the method becomes

$$x(h/2) = \frac{2q_0}{\sigma_0 + \beta_0} + \frac{\sigma_0 \phi_0 \exp(-\sigma_0 h/2)}{\alpha_0 [1 - \exp(-\sigma_0 h/2)] \phi_0} + \sigma_0 \quad (3-26)$$

The $\alpha_0, \alpha_1, \beta_0, \beta_1, q_0, q_1$, and Ψ_0 are evaluated as before from the values available at $t = 0$ and $t = h/2$ and;

$$x(h) = \frac{2q(h)}{\sigma(h) + \beta(h)} + \frac{2\phi(h/2)}{\Delta(h/2) + \sigma(h/2)} + \frac{\Delta(h/2) \Psi_0 \exp[-h \Delta(h/2)]}{\alpha(h/2) \{1 - \exp[-h \Delta(h/2) \Psi_0]\} + \Delta(h/2)} \quad (3-27a)$$

When Δ^2 is negative, the solution must be modified to

$$x(h) = \frac{2q(h)}{\sigma(h) + \beta(h)} + \frac{\Delta(h/2) \tan \left\{ \arctan[2\alpha(h/2) \Psi_0 + \sigma(h/2)/\Delta(h/2)] - 1/2 \Delta(h/2) t \right\} - \sigma(h/2)}{2\alpha(h/2)} \quad (3-27b)$$

The best value of βh or σh to divide the region of applicability of the two methods was studied by sample computations, but results were not appreciably better than with the basic algorithm.

SECTION IV

RESULTS FROM COMPUTATIONAL MODEL

A. Introduction

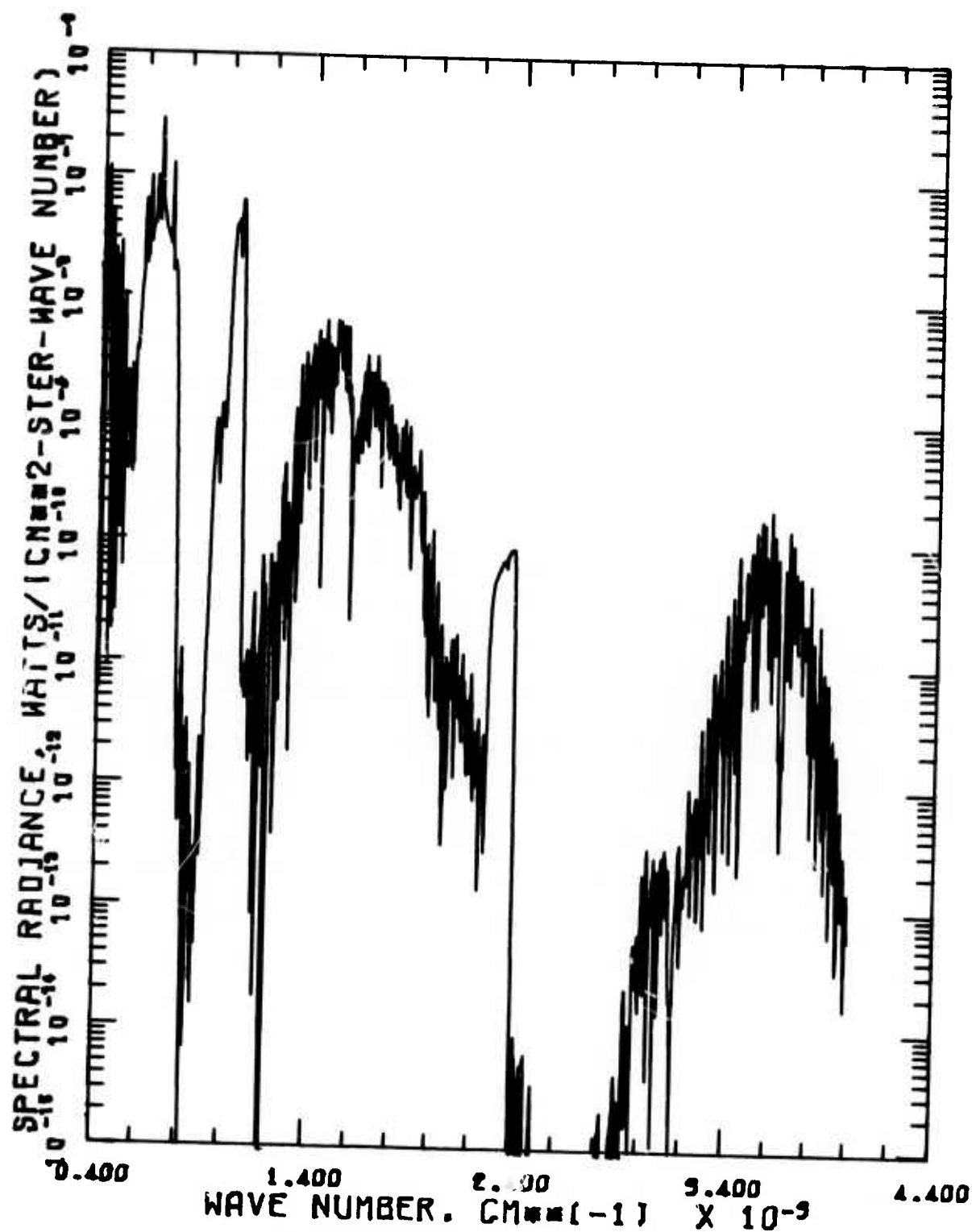
The revised high altitude spectral radiance programs can produce spectral radiance profiles for wavelengths between 2.5 and 25 micrometers or between 400 and 4000 wave numbers. Results are presented here based on estimated abundance profiles of the four species CO_2 , H_2O , O_3 and NO . The temperature and pressure profiles used were taken from the U.S. Standard Atmosphere, 1962. Upwelling terrestrial and lower atmosphere radiances are assumed to be those corresponding to a black body source at the 60 km temperature.

Spectral radiance plots are shown for typical tangent heights for day and night conditions. Features of the spectral radiance curves are explained with the aid of altitude profiles for total band radiances of individual vibrational-rotational bands.

B. Limb-Viewing Spectral Radiances

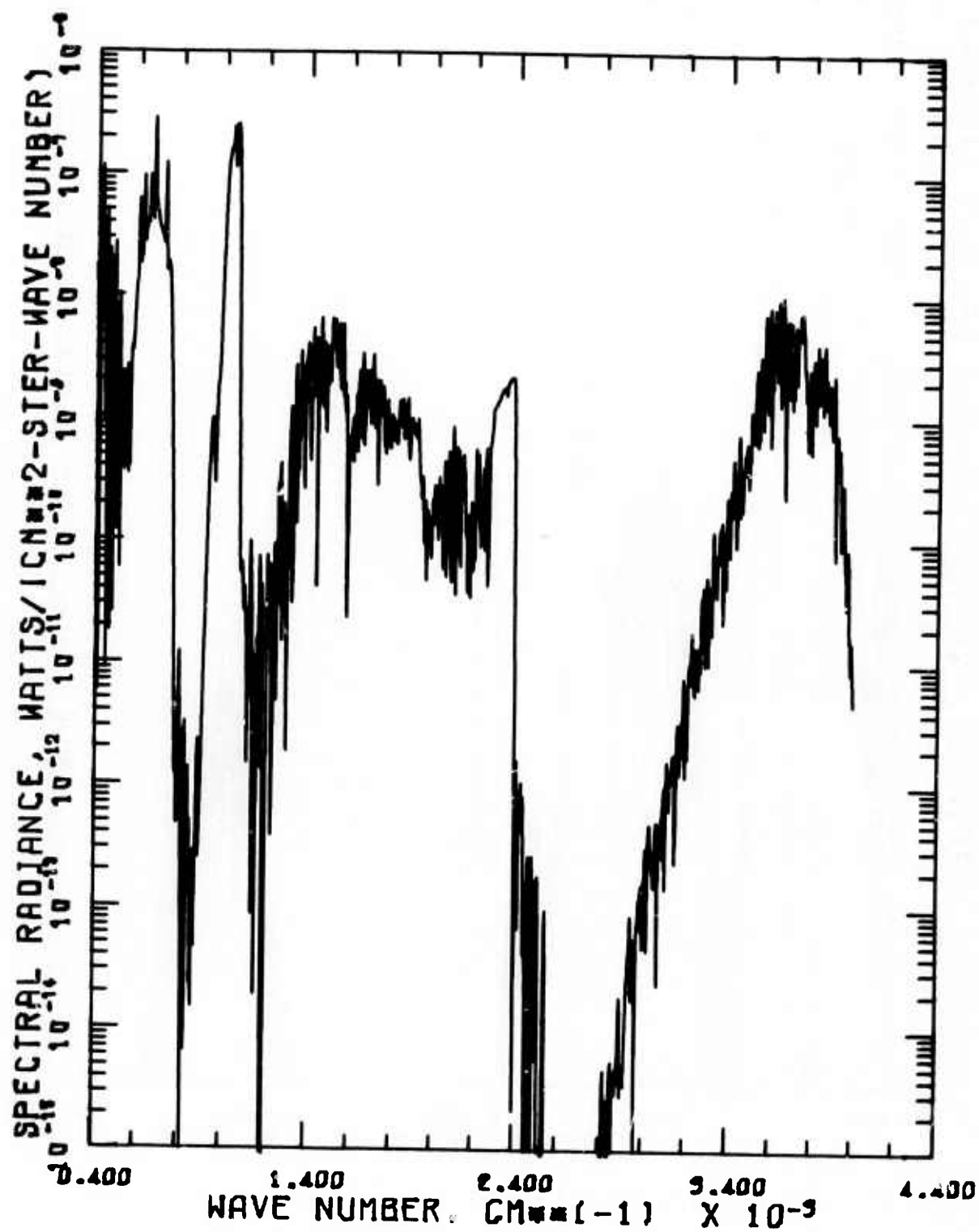
Representative limb viewing radiance profiles are shown in Figures IV-1 through IV-6. These are based on the concentration profiles of Section III, except that the experimental curve of Roble and Hays (1974) has been used for night time ozone and a constant mixing ratio has been used for CO_2 . The temperatures and number densities used are those of the U.S. Standard Atmosphere, 1962.

The results shown are quite different from those of Degges (1972) for many of the carbon dioxide bands, where the earlier version of the program predicted appreciably lower radiance values at high altitudes. The night time ozone radiance



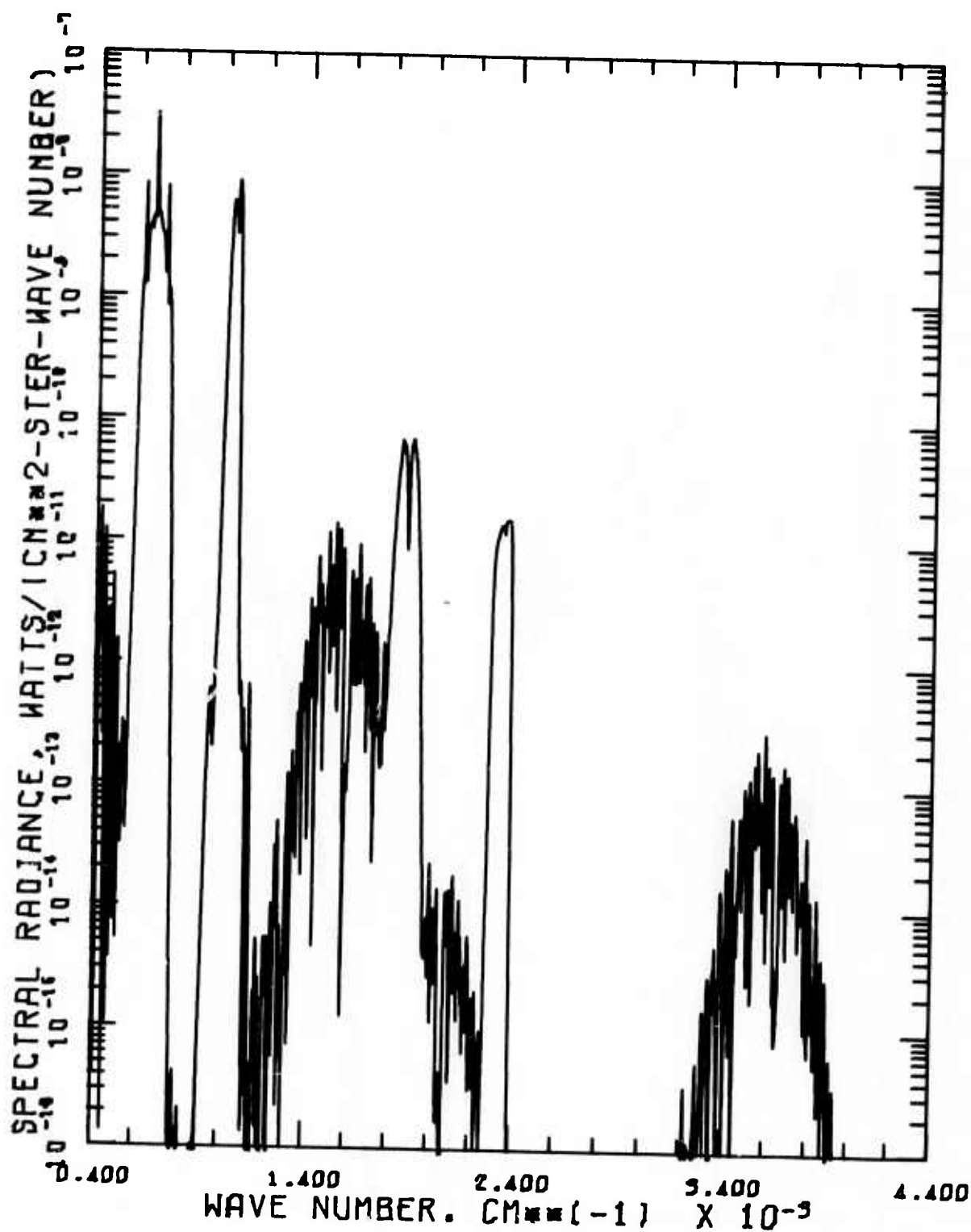
Night Limb Viewing Spectral Radiance,
400 to 4000 cm⁻¹, 60 km Tangent Height

FIGURE IV-1



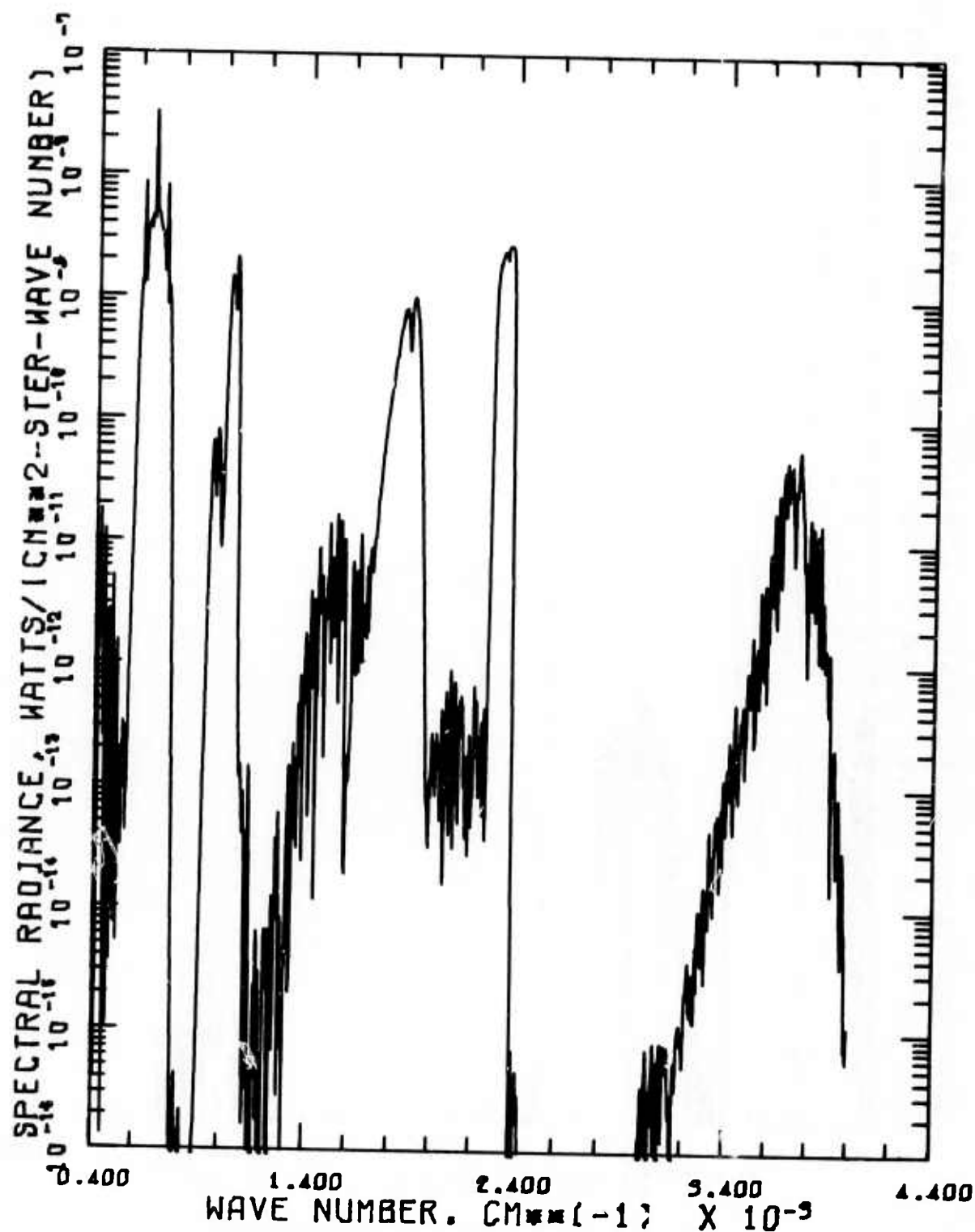
Day Limb Viewing Spectral Radiance,
400 to 4000 cm⁻¹, 60km Tangent Height.

FIGURE IV-2



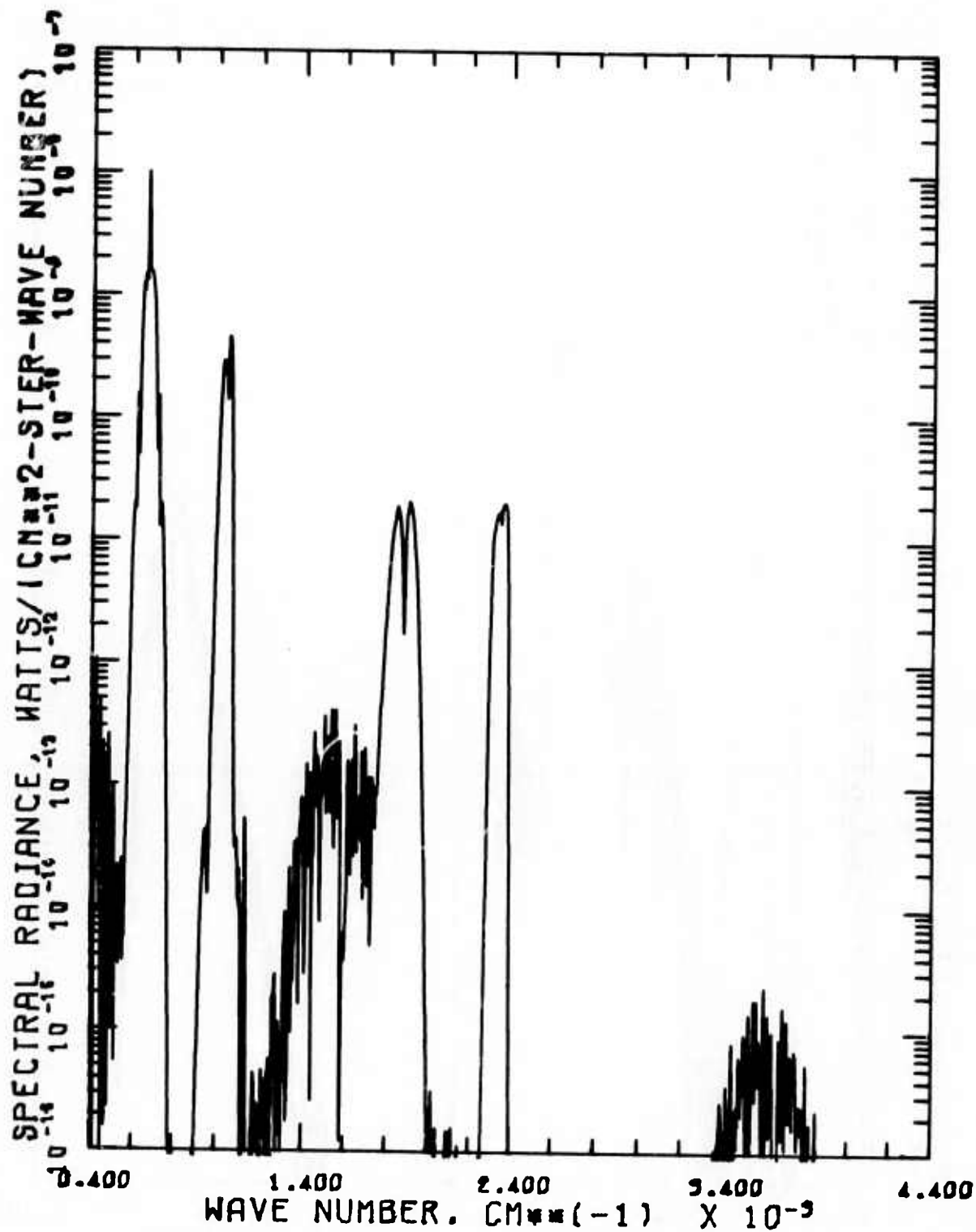
Night Limb Viewing Spectral Radiance,
 400 to 4000 cm^{-1} , 80 km Tangent Height.

FIGURE IV-3



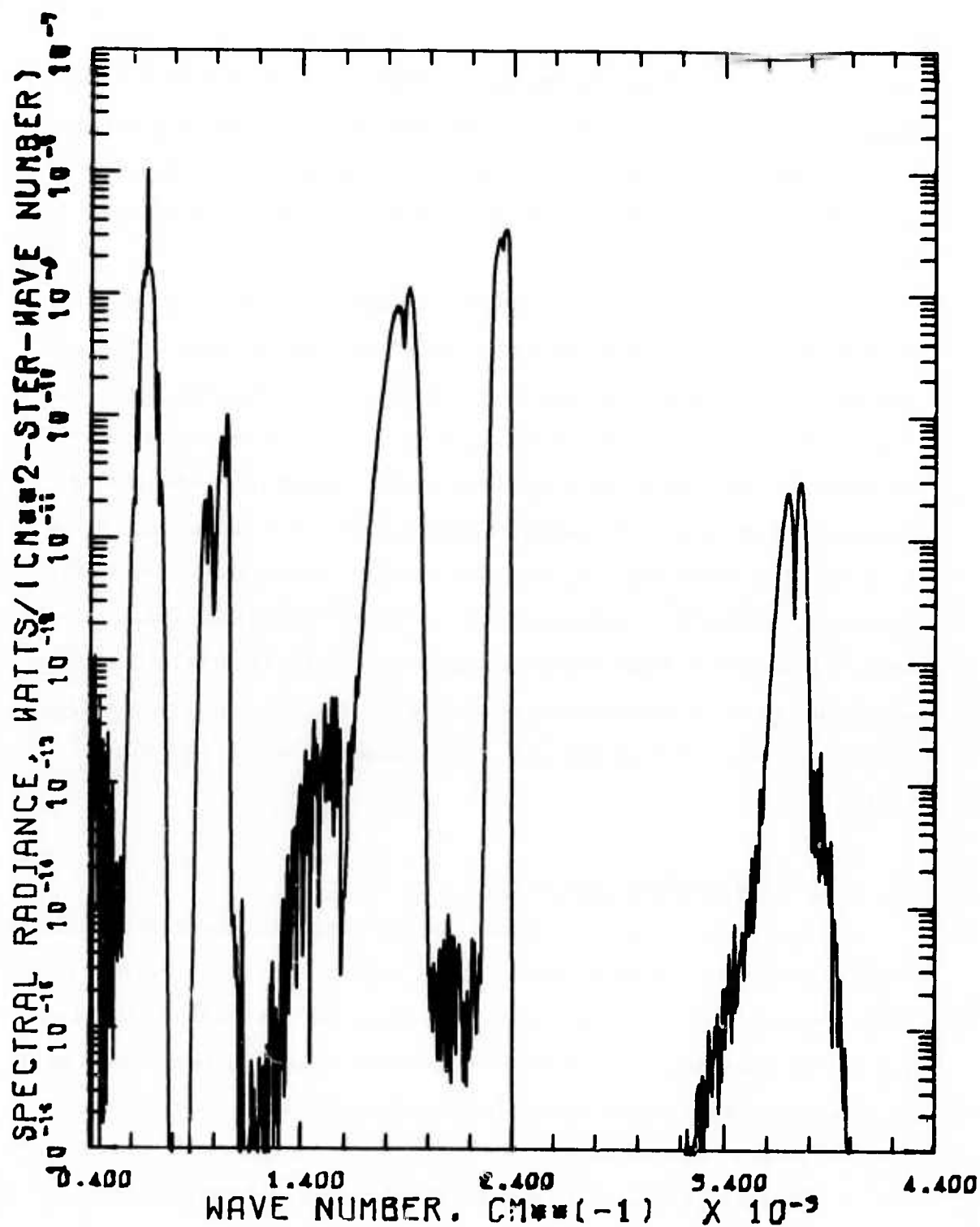
Day Limb Viewing Spectral Radiance,
400 to 4000 cm⁻¹, 80 km Tangent Height.

FIGURE IV-4



Night Limb Viewing Spectral Radiance,
400 to 4000 cm^{-1} , 100 km Tangent Height.

FIGURE IV-5



Day Lamb Viewing Spectral Radiance,
400 to 4000 cm⁻¹, 100 km Tangent Height.

FIGURE IV-6

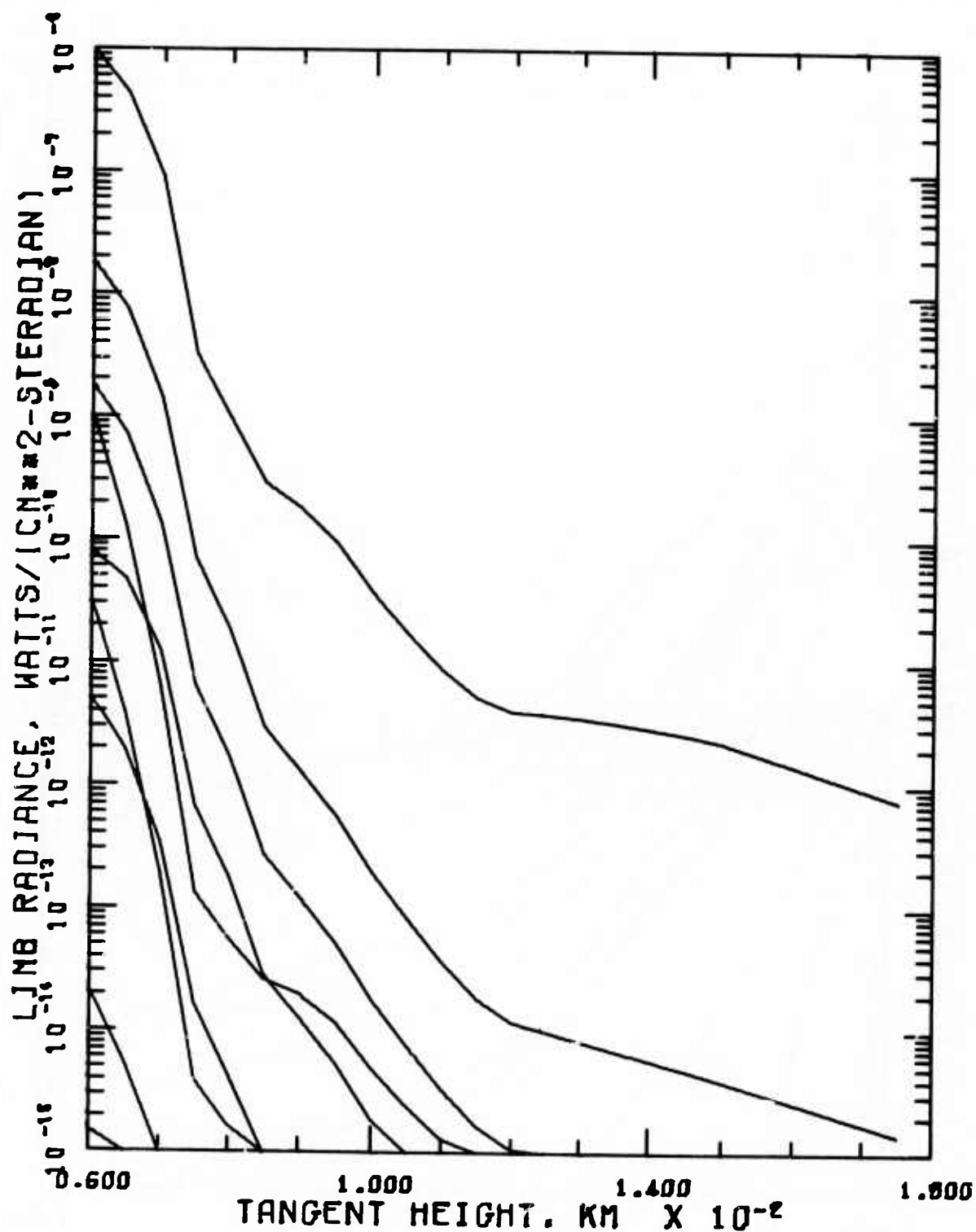
values are also higher in spite of a reduction in total column count (molecules/cm²) above 60 km. The differences in the CO₂ values are primarily because the early program did not correctly integrate the radiation field produced by molecules radiating above 60 km.

Comparison of day and night profiles for a given tangent height shows that the low energy (small wave number and long wave length) band radiances do not vary appreciably during the day. The high altitude high energy bands, however, do vary in intensity by as much as two orders of magnitude as the result of resonant and fluorescent emission following absorption of solar radiation. This is shown clearly in the CO₂ 4.3 micrometer bands and in the water vapor complex at 2.7 micrometers. A faint indication of this effect is visible in the 5.4 micrometer nitric oxide fundamental where the day time curve is broadened because of the fluorescent contribution from absorption of sunlight at 2.7 micrometers and in the ultra-violet.

C. Individual Band Radiances

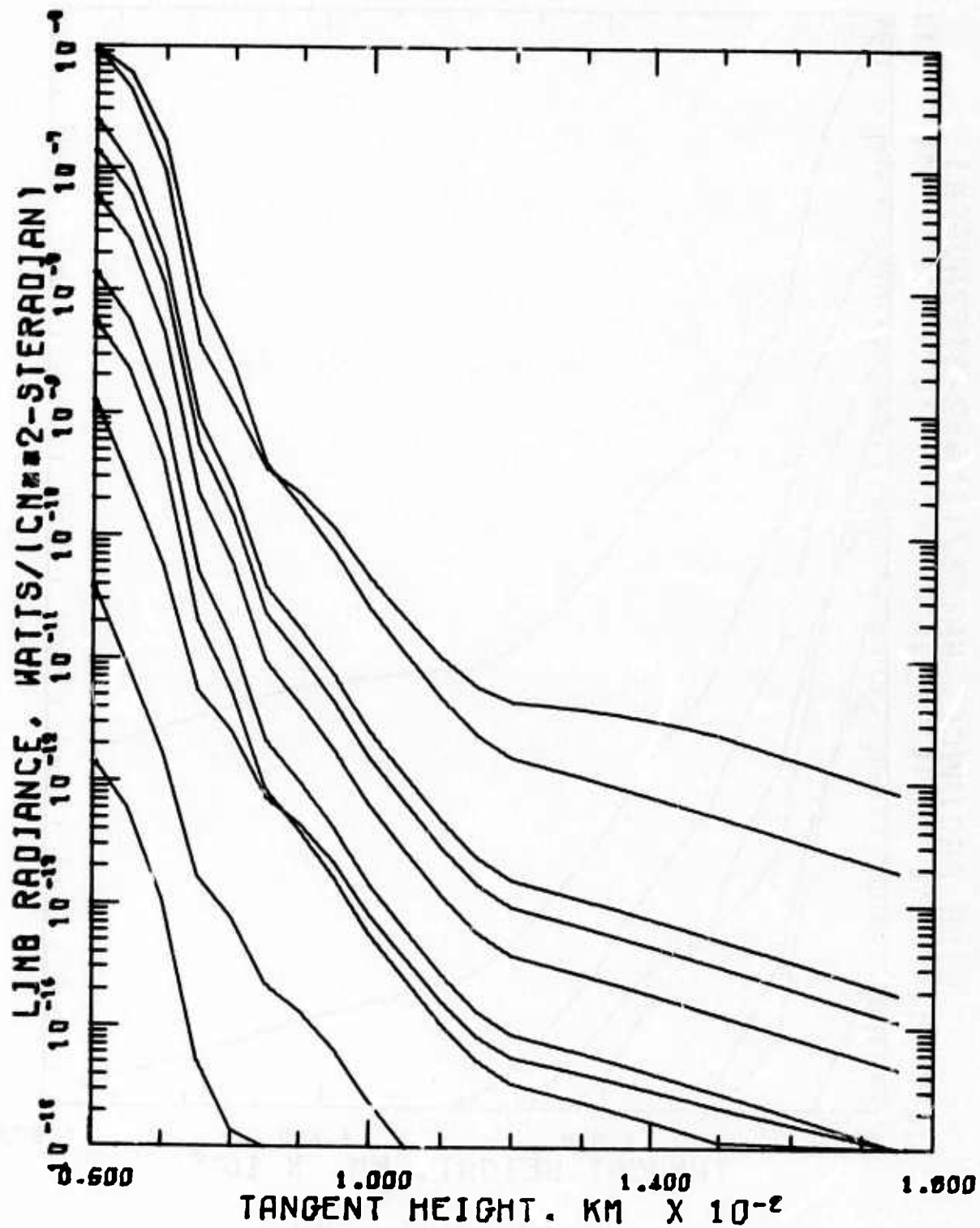
For some purposes, it may be more convenient to have available the total radiance of an individual band rather than the spectrum of the region where the band is located. This may aid in making allowances for species abundances different from those assumed in a computation or in assigning an experimentally observed radiance value to one species rather than another.

Figures IV-7 and IV-8 show the day and night total band radiances for the ten water vapor bands included in the spectra of Figures IV-1 through IV-6. The 6.3 micrometer ν_2 band is the



Night Limb Viewing Total
 Band Radiance Values for Water Vapor Bands

FIGURE IV-7



Day Limb Viewing Total
 Band Radiance Values for Water Vapor Bands

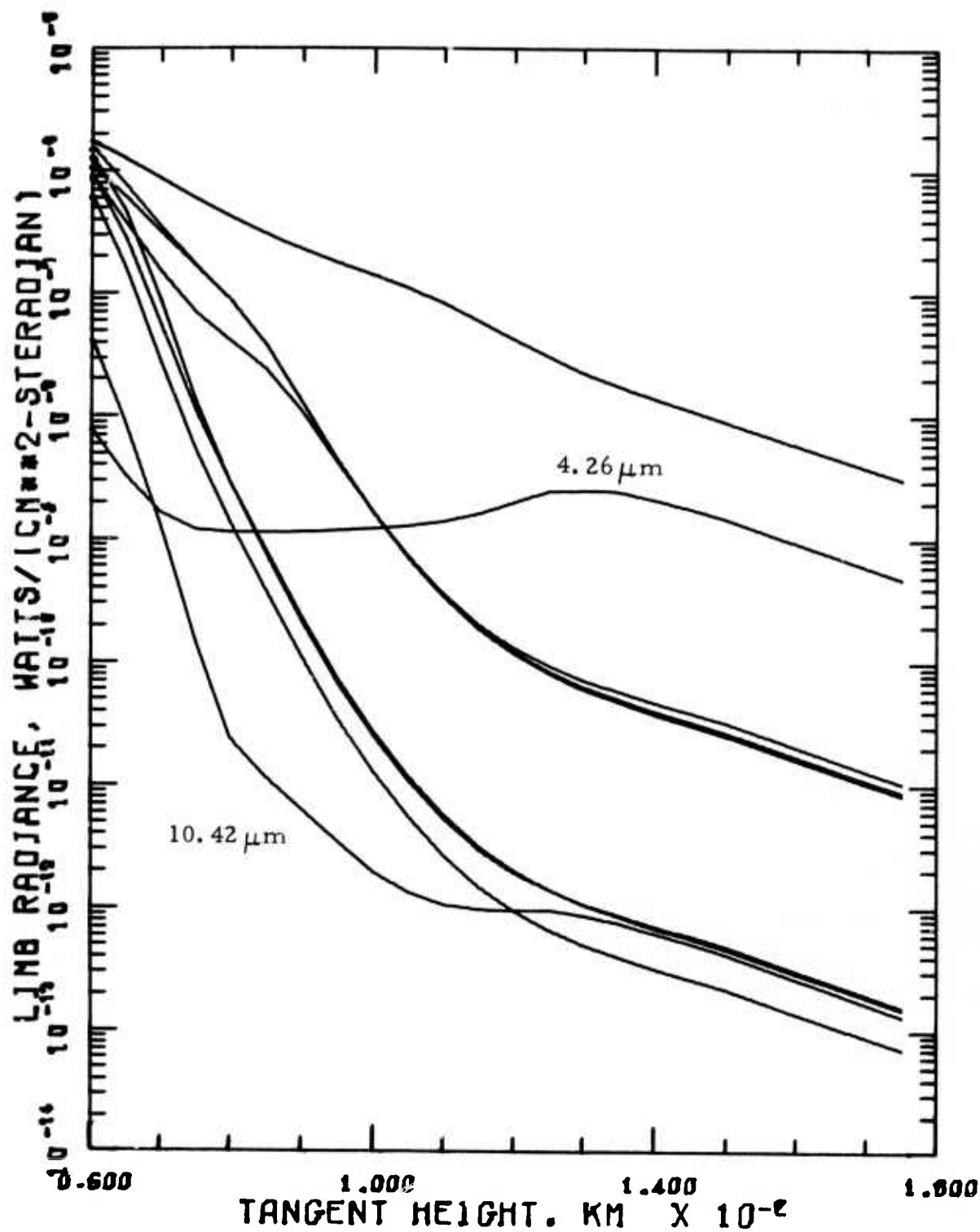
FIGURE IV-8

strongest, day or night. During the day, the ν_3 band at 2.66 micrometers strongly absorbs solar radiation and becomes almost as bright at a tangent height near 90 km. At night this band is nearly four orders of magnitude fainter.

Figures IV-9 and IV-10 show night and day limb radiance values for seven bands of the CO_2 15 micrometer band complex, the 4.3 micrometer ν_3 band and one of the two fluorescent bands originating from the ν_3 state, the 10.42 micrometer 00011 - 10001 Band. The 15 micrometer band radiances vary little between day and night. During the day, however, the radiance of the 4.3 micrometer band rises from its night value of between 10^{-9} and 10^{-8} watts/cm²-ster to a value of between 10^{-8} and 2×10^{-7} watts/cm²-ster. This band is thick in the limb viewing geometry, and most of the increase is due to increased vibrational temperatures at altitudes above 90 km. The 10.41 micrometer band, which has much lower optical thickness, gives a better indication of the altitudes at which the solar excitation is important. The 60 km value is about 4×10^{-8} watts/cm²-ster day or night. Figure IV-11 shows night limb radiance values for the same CO_2 bands when the mesopause temperature is raised to 230 K. The main effect is to double or triple the band radiance values, indicating the importance of the temperature profile in computing radiance values.

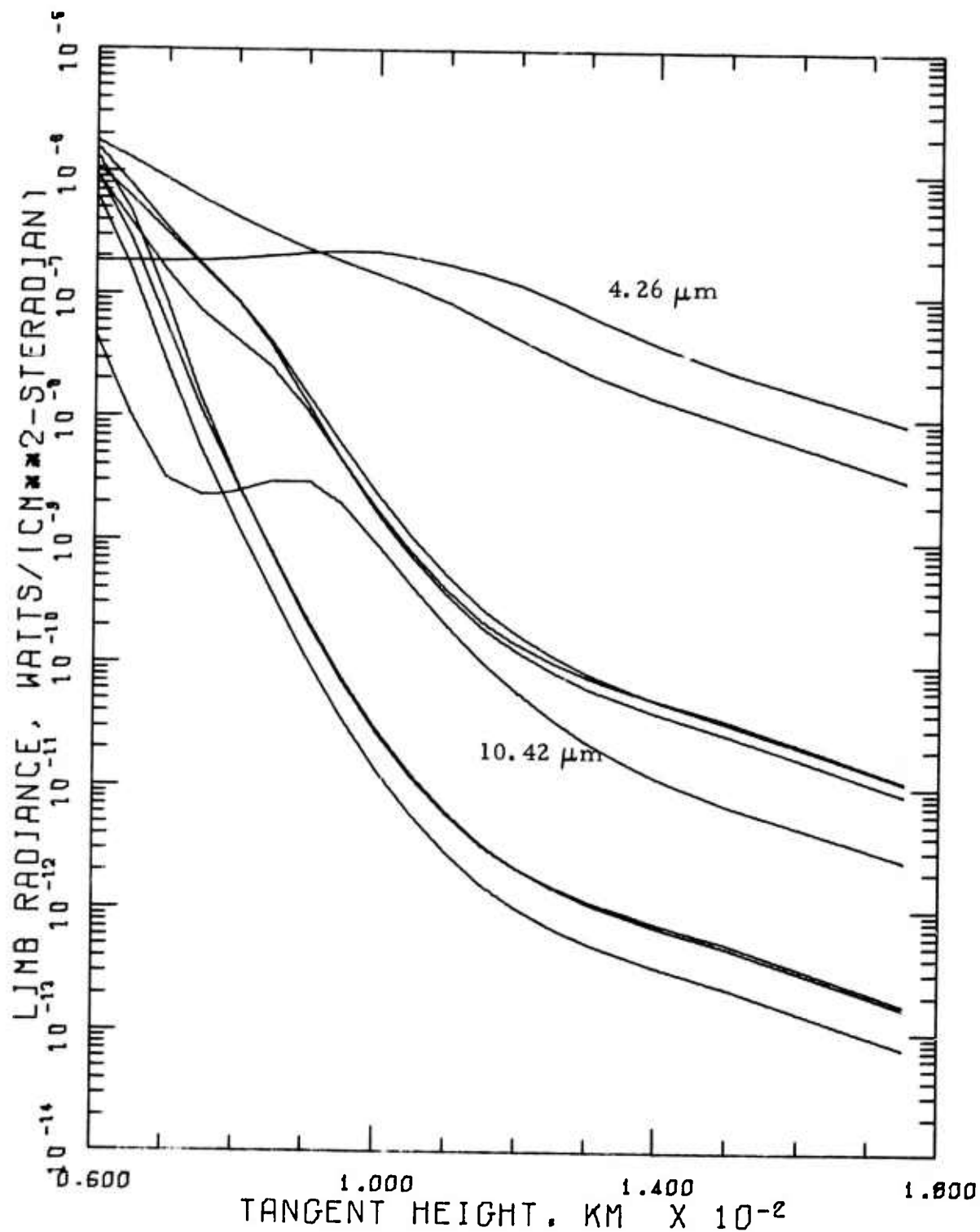
D. Comparison with Observations

A limited amount of data from the ICECAP program is available for comparison with the results of the radiance computer program. Figure IV-12 compares peak spectral radiance values for the 15 micrometer band measured by Stair, et al (1974) with those



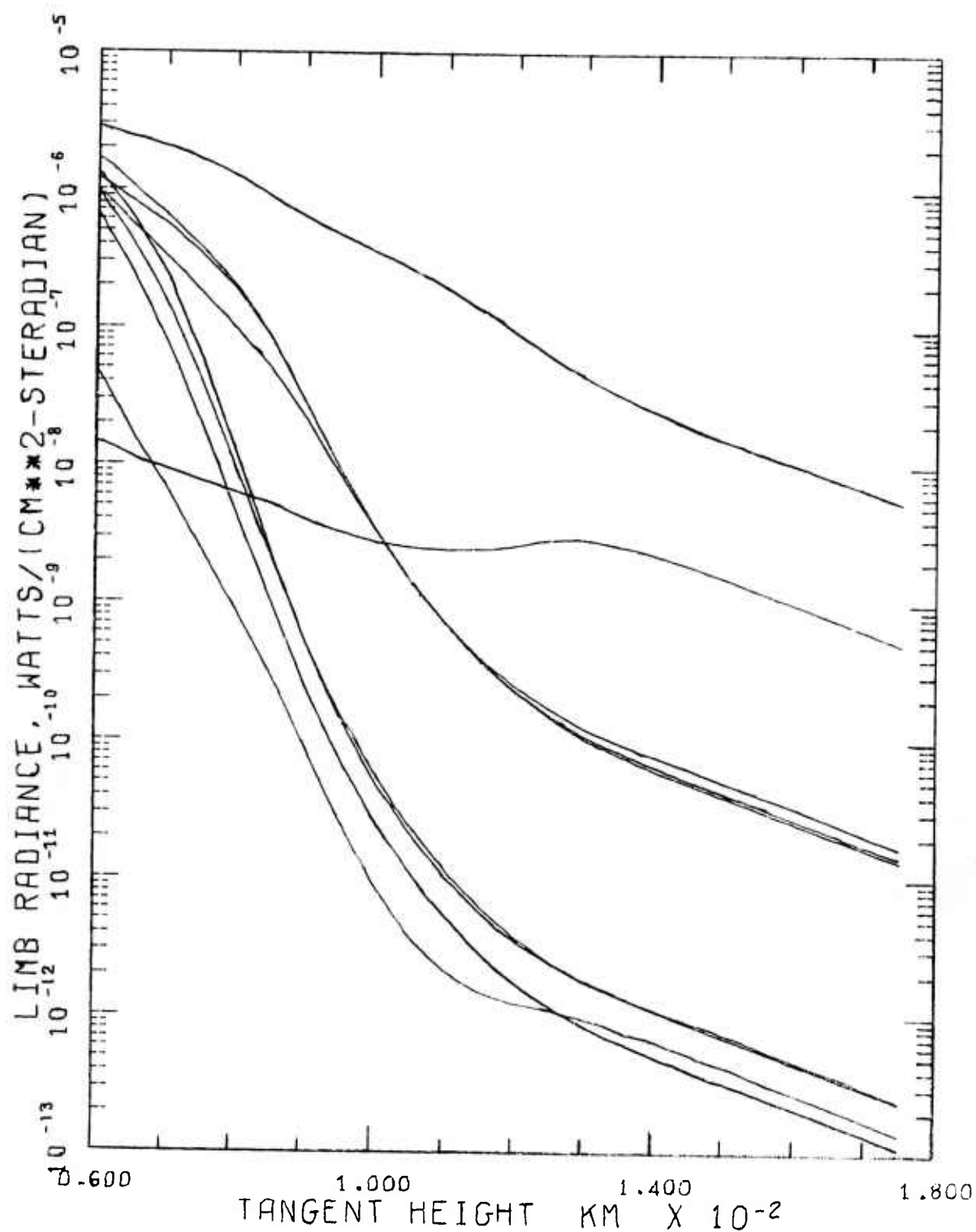
Nighttime Limb Radiance, CO₂
 15 μm Bands, 10.42 μm Band and 4.26 μm Band.

FIGURE IV-9



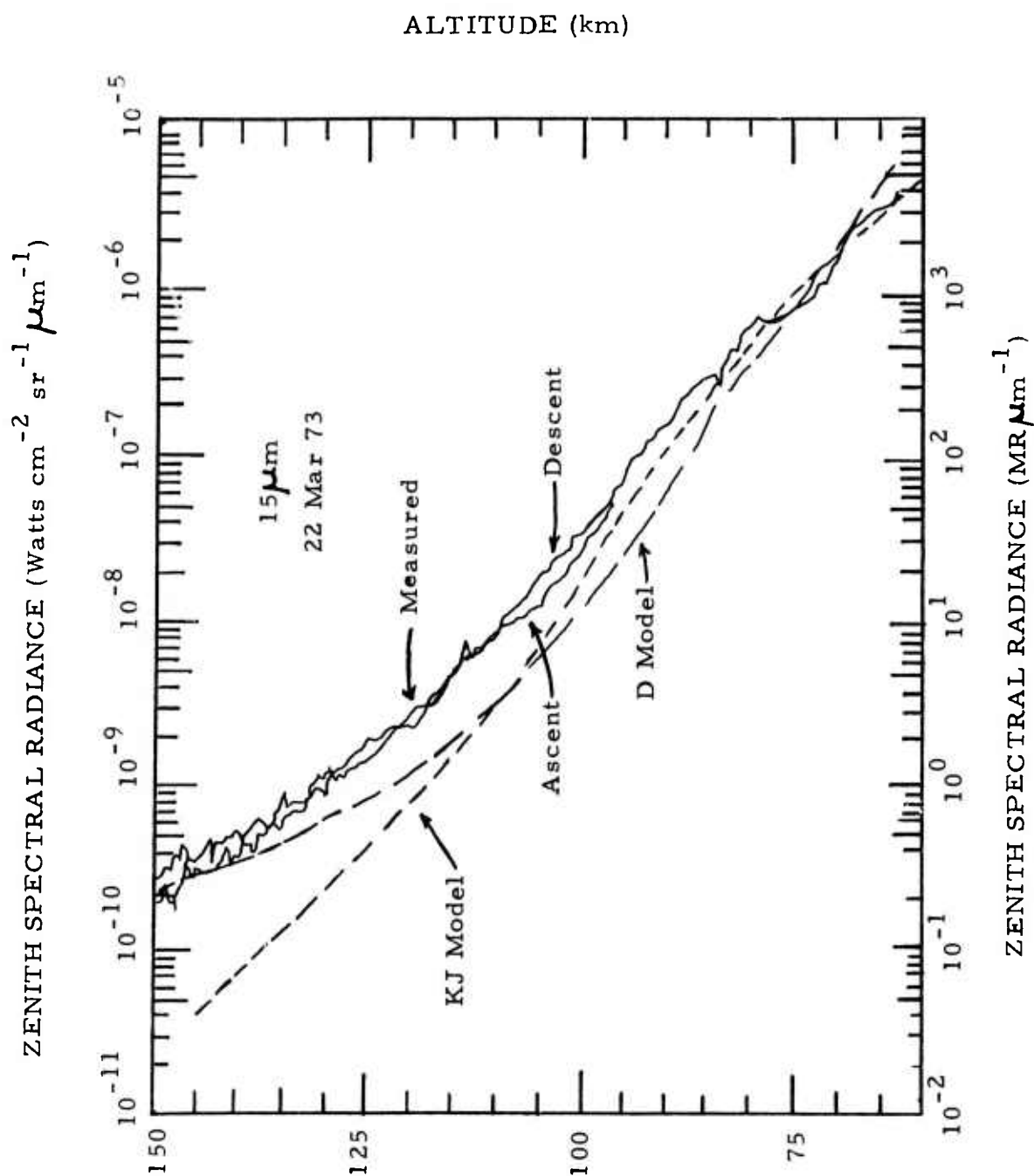
Daytime Limb Radiance, CO₂
 15 μm Bands, 10.42 μm Band and 4.26 μm Band.

FIGURE IV-10



NIGHTTIME LIMB RADIANCE, CO₂
 15 μ m BANDS, 10.42 μ m BAND and 4.26 μ m BAND
 230 K MESOPAUSE

FIGURE IV-11



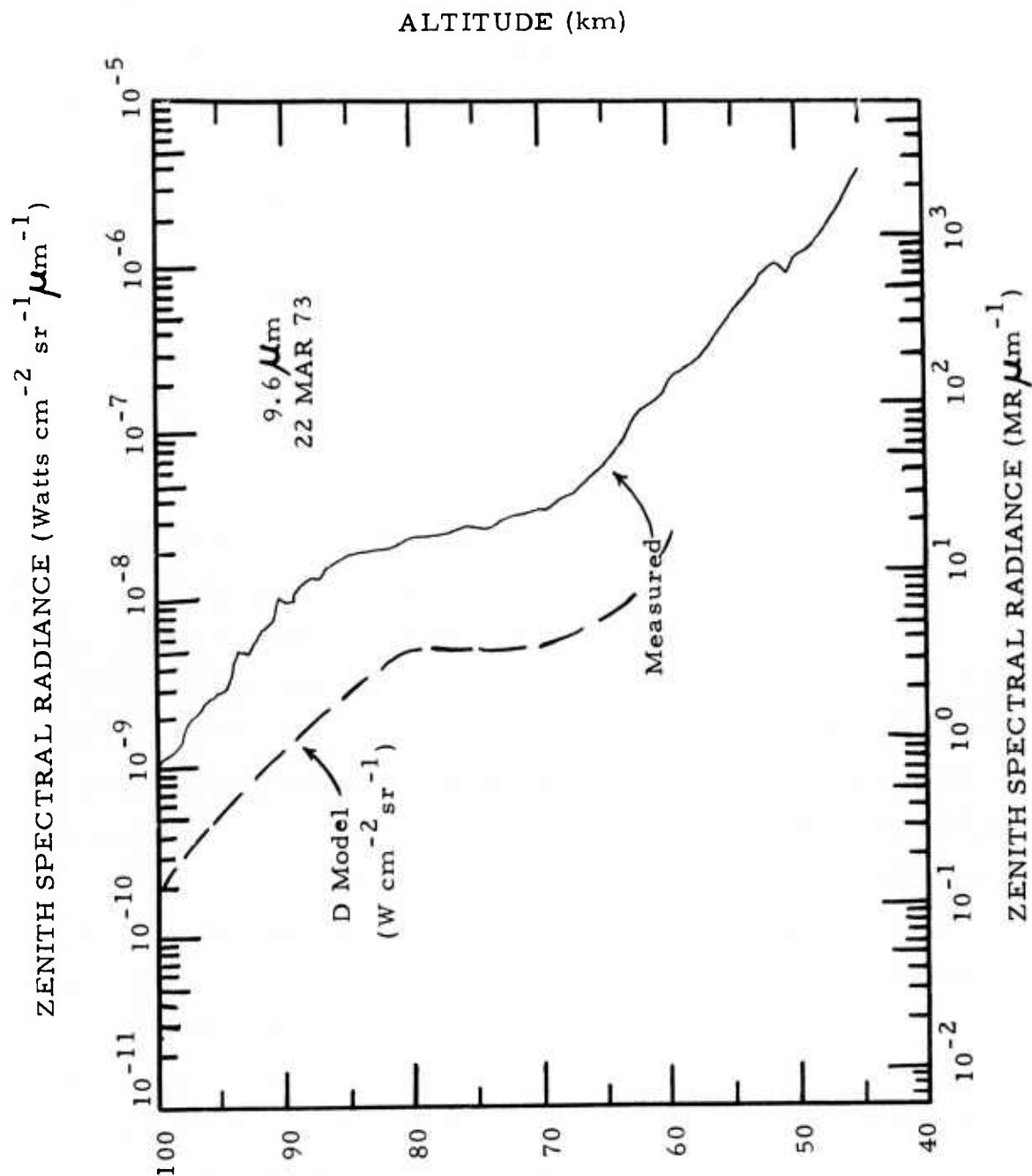
Zenith peak spectral radiance at $15\mu\text{m}$ measured with LWIR spectrometer aboard rocket flown at Poker Flat, Alaska on 22 March 73 compared to theoretical model. The solid curve is the measured profiles (ascent and descent) while the dashed curves show model calculations of Kumer and James (KJ) and Corbin and Degges (D).

computed by the radiance program (D Model) using the U.S. Standard Atmosphere, 1962 temperature profile with 180 K mesopause temperature and that computed by J. B. Kumer (K. J. Model) using the Kumer and James (1973) model radiance program. The differences between the results of the two computer programs are due principally to differing temperature profiles and assumed CO₂ mixing ratios. The degree of agreement between the two models and the experimental data give an indication of what can be expected from use of the computer programs and the need to improve both the computational algorithms and knowledge of atmospheric composition.

Figure IV-13 compares the radiance model prediction with the data of Stair, et al (1974), this time for the ozone ν_3 band. The amount of ozone used for the calculation is optically thin in the upward direction, and doubling the amount would double the computed radiance. The effective width of the observed ozone band is about one-third micrometer, and the plotted experimental data agrees with the measurement to within a factor of two. The shape of the observed radiance curve supports the accuracy of the ozone measurement of Hays and Roble and their interpretation that their observed ultraviolet absorption is due to ozone and not a mesospheric aerosol layer. Figure IV-13, as well as Figure IV-12, shows that at least some results of the radiance program are in agreement with measured radiances, and suggests that with more accurate data on atmospheric temperature and composition, observations will either confirm model predictions or show how modeling algorithms must be modified.

E. Model Evaluation

The most important general areas of investigation in this research effort have been (a) the chemistry and spatial variation



Zenith peak spectral radiance at $9.6\mu\text{m}$ measured with LWIR spectrometer aboard rocket flown at Poker Flat, Alaska on 22 March 73 compared to theoretical model. The solid curve is the measured profile while the dashed curve shows the D Model calculations in $\text{watts cm}^{-2} \text{ster}^{-1}$.

FIGURE IV-13

of atmospheric species important to infrared radiation and (b) the improvement of models for the transport of infrared radiation.

Section III dealt with atmospheric composition and modifications to the chemistry program written during a previous research effort (Degges, 1972). This program remains limited in its usefulness to short time extrapolation from a given set of atmospheric composition profiles. It can be used to give limited information on such problems as auroral chemistry, but requires knowledge of the limitations imposed by the limited chemistry set and uncertainties in global transport of such important species as atomic oxygen.

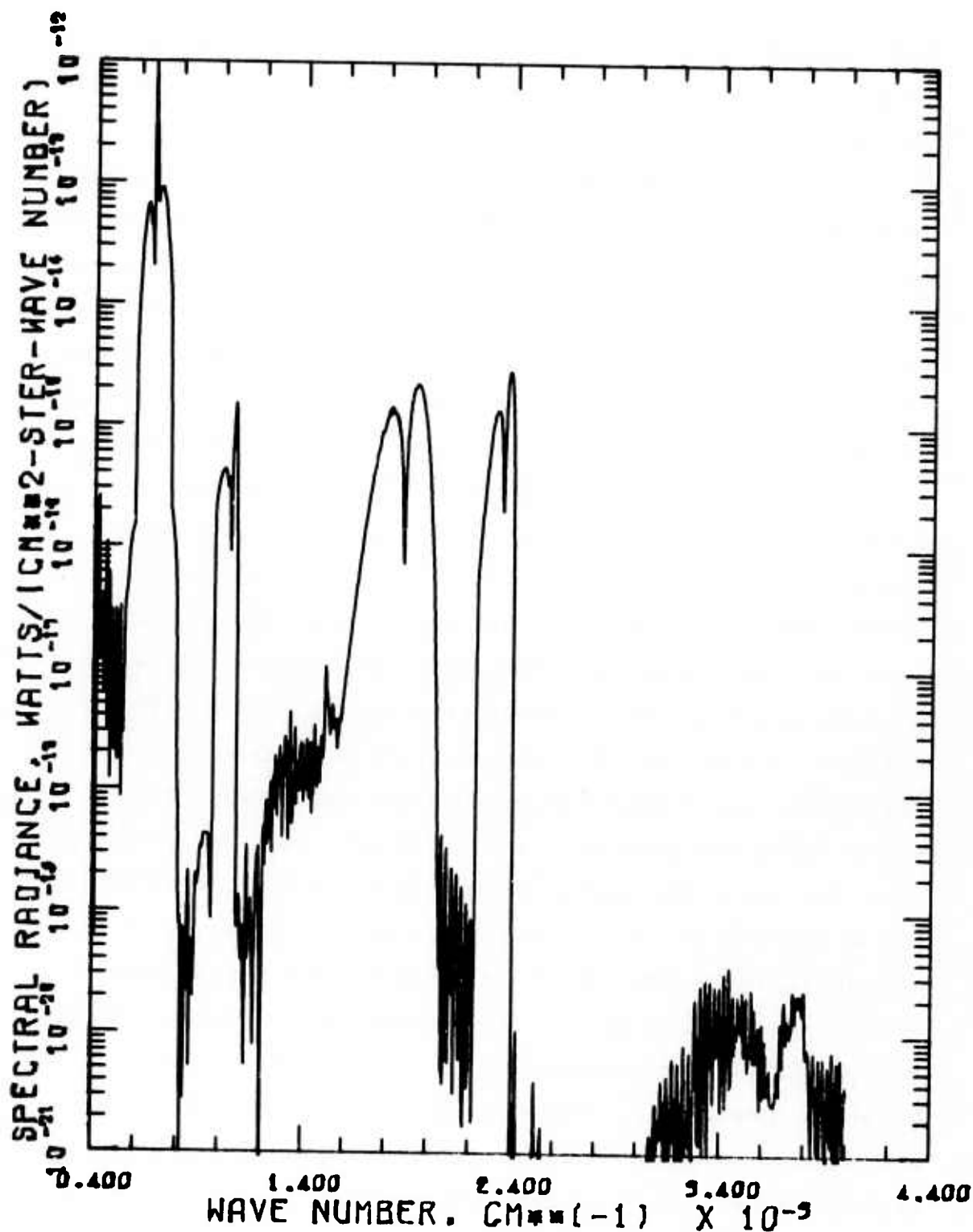
More important advances have been made in the radiative transport program. A serious programming error has been corrected, and an improved formulation of the transport problem has been coded. The program produces results which agree with a limited amount of observational data. The agreement with the carbon dioxide radiance model of James and Kumer (1973) is believed to be satisfactory. There remain areas in which results were not as good as those anticipated when the work was initiated.

The program for computing band radiances requires an excessive amount of computer time for bands that are optically thick in the upward direction above the altitude at which collisions are important in determining vibrational populations. The spectral radiance program is much slower now that a relatively complete set of spectral lines is used for the water vapor and ozone bands. The first of these problems can be resolved by using a matrix inversion to obtain a first approximation to the vibrational populations of the optically thick bands, as is done in the program developed by James and Kumer. The second problem is a result of trying for completeness,

and a smaller set of lines may be selected and used for some purposes, using more complete results as a guide to what may be safely omitted.

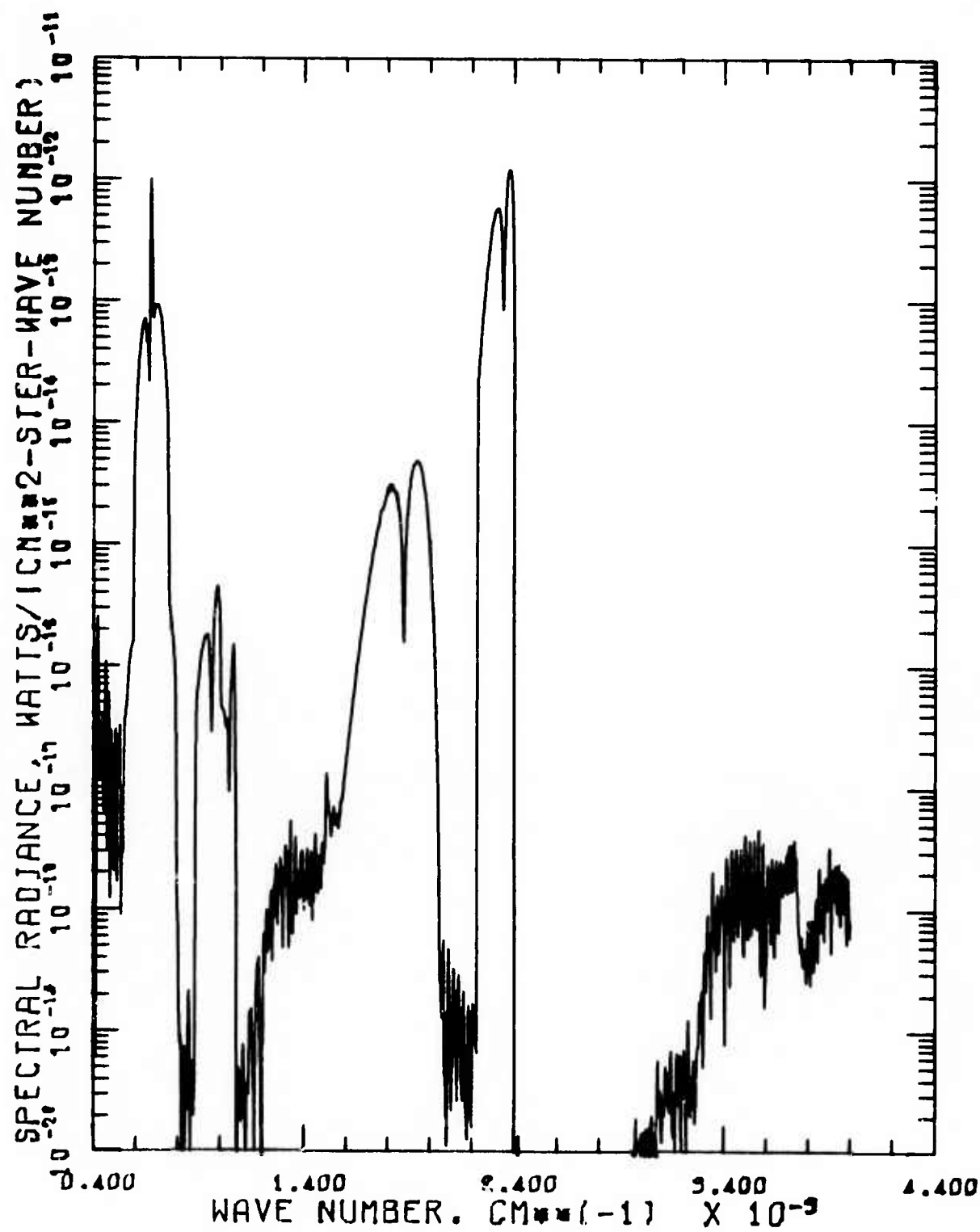
The program could be improved in some other ways by adding features from programs such as that of Whiting, et al (1969), which was written to compute line-by-line spectra of diatomic molecules. Use of this program with either of the Voight profile subroutines used in the current research effort would permit improved calculation of limb radiances, provided composition data are sufficiently accurate to justify the additional programming effort and computer time.

Finally, we use Figures IV-14 and IV-15 to illustrate one remaining problem. These figures give night and day spectral radiance values for a limb view with a tangent height of 500 km. Comparison with Figures IV-1 through IV-6 shows that the band widths are appreciably wider than for the lower atmosphere where the temperature is lower. The program assumes that the effective radiation received from the lower atmosphere and from the lower parts of the upper atmosphere is such as to produce a constant vibrational temperature above 110 or 120 km. Above these altitudes, collisions play no part and excitation is entirely by radiative transfer. The widening of the bands at very high altitudes will permit absorption of radiation in the wings of the band, and this effect is not properly accounted for in the program. Additionally, at an altitude of 500 km, it is probable that the rotational temperature is not in equilibrium with the kinetic temperature. Further work is required to investigate the actual rotational temperature when collisions are not sufficiently rapid to maintain rotational temperature in equilibrium with kinetic temperature.



Night Limb Viewing Spectral Radiance,
400 to 4000 cm⁻¹, 500 km Tangent Height.

FIGURE IV-14



Day Limb Viewing Spectral Radiance,
400 to 4000 cm^{-1} , 500 km Tangent Height.

FIGURE IV-15

SECTION V

HIGH ALTITUDE RADIANCE PROGRAMS

The high altitude (>60 km) radiance program set includes four programs, LOWRAD, BCKGND, SPCTRA and TRYCRT. Each program may be used separately or in appropriate combination with one or more of the others within the CDC 6600 operating system.

LOWRAD is used only to provide an approximation to the spectral radiance in the upward direction from the lower atmosphere. Input to LOWRAD is from two separate files, TAPE 1 which holds the premanent data and data for five model atmospheres and TAPE 5 = INPUT which directs the choice of one of the five atmospheres or another atmosphere, in which case data for this atmosphere must also be on TAPE 5. Printed output is written to TAPE 6 = OUTPUT and output in a form suitable for use by BCKGND is written to TAPE 2, which may be a temporary or permanent disc file or a magnetic tape.

BCKGND computes vibrational populations and total band radiances for an earth's limb viewing geometry at 5 km intervals between 60 and 120 and at 25 km intervals between 120 and 500 km. Control information is read from TAPE 5 = INPUT and permanent data is read from TAPE 1. Low altitude spectral radiances are read from TAPE 2. Atmospheric composition at 2 km intervals between 60 and 150 km and at 5 km intervals between 150 and 700 km may be read either from a sample transferred from the UPDATE set to TAPE 1 or from TAPE 5. Output for printing is written to TAPE 6 = OUTPUT and to TAPE 3 for storage or for use as input to program SPCTRA.

Preceding page blank

SPCTRA computes spectral radiances corresponding to the total band radiances output by BCKGND. Control information is read from TAPE 5 = INPUT. Permanent data is read from TAPE 1 and the results of the BCKGND computation are read from TAPE 3. Output data is sent to TAPE 6 = OUTPUT for printing and to TAPE 4 for use by the plotting program. Optional output of unfiltered spectral radiances may be placed on TAPE 7 and saved for later use.

TRYPEN and TRYCRT plot spectral radiance curves using values computed by program SPCTRA. TRYCRT produces microfilm output; TRYPEN uses a pen plotter.

The programs are listed and described below.

Program LOWRAD

LOWRAD is used to provide an approximation to the spectral radiance in the upward direction from the lower atmosphere. It is based on the computer program, LOWTRAN 1, written by J. E. A. Selby of AFCRL. LOWTRAN 1 provides numerical values based on the atmospheric transmission model of McClatchey, et al (1970).

LOWTRAN 1 is capable of computing transmittances with 20 wavenumber resolution at wavenumbers between 350 and 40,000 cm^{-1} (0.25 to 28.5 micrometers). Computations are restricted to points with numerical value a multiple of five wavenumbers. LOWTRAN 1 uses atmospheric parameters (temperature, pressure, and composition) at one kilometer intervals between 0 and 25 km, at five kilometer intervals to 50 km, and at 70 and 100 km. Variables required at intermediate altitudes are obtained by interpolation.

The modifications to LOWTRAN 1 to make LOWRAD are simple and straightforward. Beginning at 350 cm^{-1} , transmission between 60 km and each lower level of the atmosphere is computed for 5 nadir angles. The Planck function at that wavenumber is computed for ground level temperature and the mean temperature between altitude levels used by the program. The ground level value of the Planck function is multiplied by the transmittance between ground level and 60 km altitude. This and the product of the Planck function and transmittance differences for the intermediate levels are summed to produce spectral radiance values at each of the given angles. The version of LOWRAD listed here uses the five angles $\arcsin \sqrt{(2I - 1)/10}$ with I taking values one to five. Equal weights are assigned to the radiances computed with each value of I, and the arithmetic mean is taken to be the value of the upwelling spectral

radiance. An effective radiation temperature is computed from the final spectral radiance value for use (if desired) with program BCKGND. This procedure is repeated at 5 cm^{-1} intervals until 4000 cm^{-1} (2.5 micrometers) for a total of 731 output radiance values. These output values are written both to the line printer and to a disc file for later use.

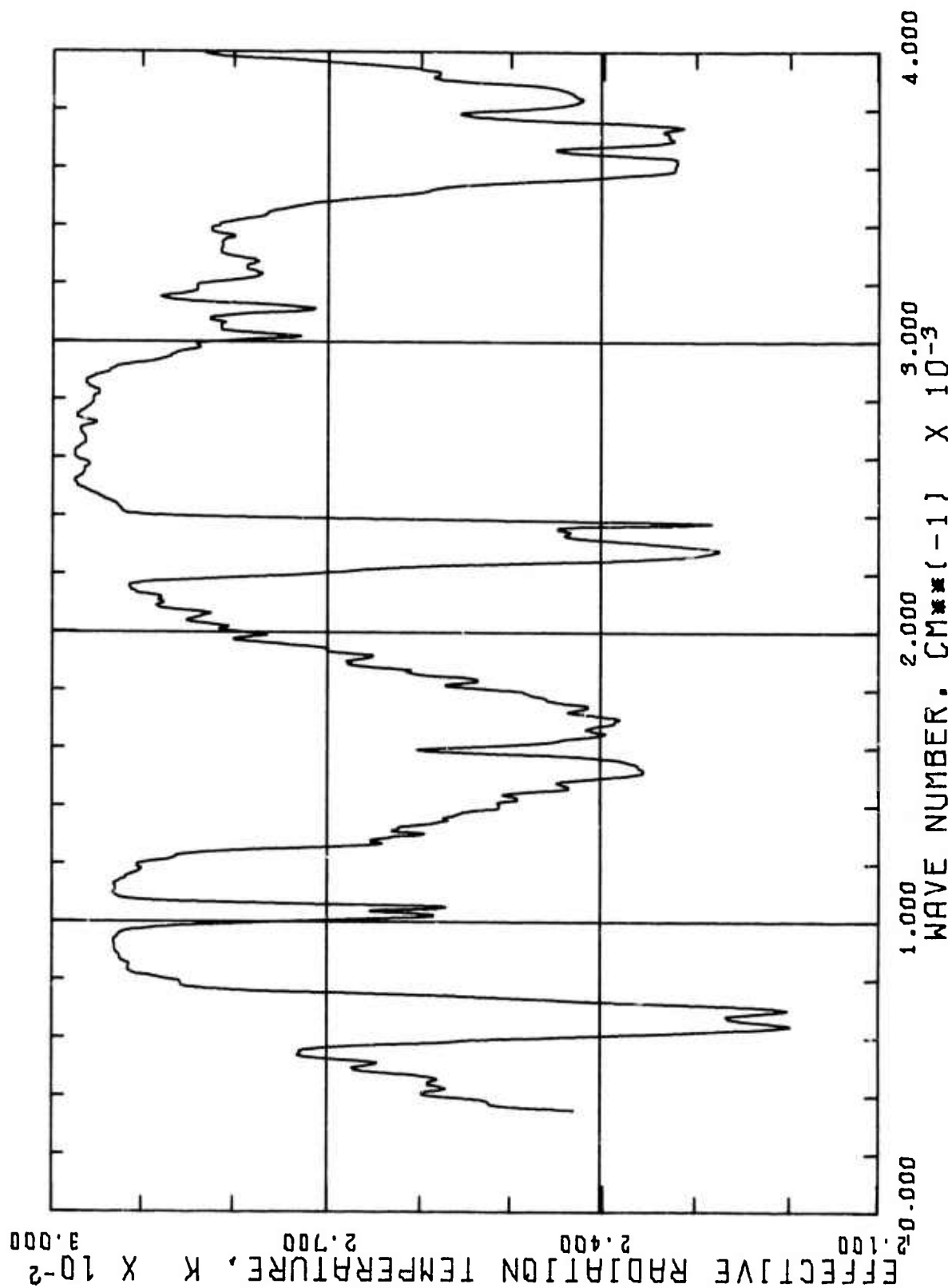
Figures V-1 through V-5 show the resulting values of radiation temperature for the five model atmospheres provided by McClatchey, et al (1970). The effects of the strong absorption bands of CO_2 , H_2O and O_3 are easily seen in the lower temperatures at the most intense parts of the bands, where a detector looking down would in effect see the cold lower stratosphere.

Table V-1 lists radiation temperature values for the five model atmospheres, (1) tropical, (2) midlatitude summer, (3) midlatitude winter, (4) sub-artic summer and (5) sub-artic winter.

The radiance values and effective radiation temperatures computed by LOWRAD are limited in usefulness by the low resolution available. A molecule in the upper atmosphere acts as its own spectrometer with a resolution comparable to its line width which is of the order of between one hundredth and one tenth of a wave number. For most bands, a better value of effective radiation temperature is that of the kinetic temperature at the altitude taken to be the base of the high altitude region. This is 60 km for the high altitude radiance program BCKGND.

Input to LOWRAD is from two separate files, TAPE 5, which holds permanent transmission data and data for five model atmospheres and TAPE 4 which directs the choice of one of the five atmospheres or another atmosphere, in which case data for this atmosphere must also be on TAPE 5. Printed output is written to TAPE 6 = OUTPUT and

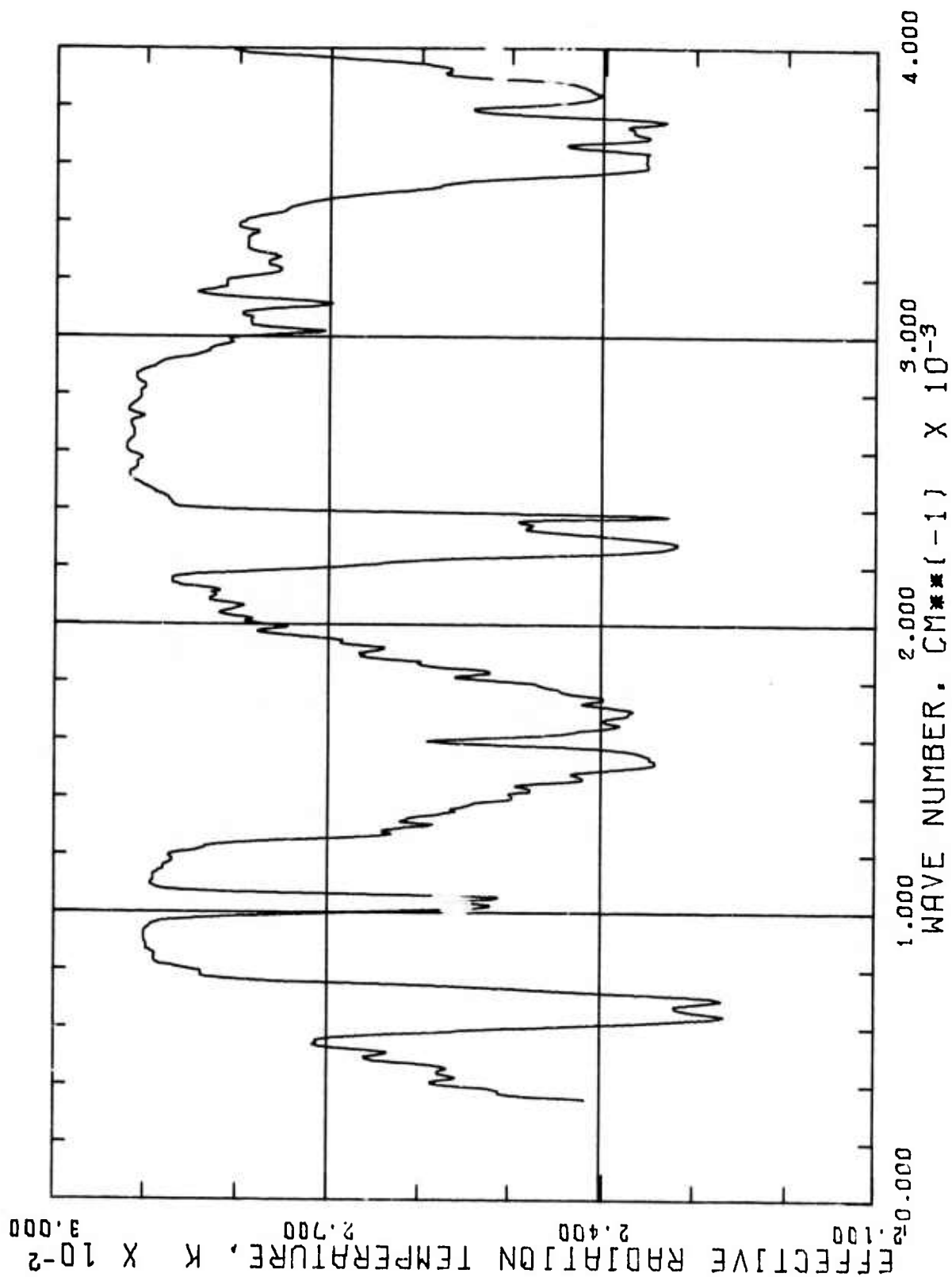
output in a form suitable for use by BCKGND is written to TAPE 2, which may be a temporary or permanent disc file or a magnetic tape.



Lower Atmosphere Radiation Temperature

For Tropical Model Atmosphere

FIGURE V-1



Lower Atmosphere Radiation Temperature
For Midlatitude Summer Model Atmosphere

FIGURE V-2

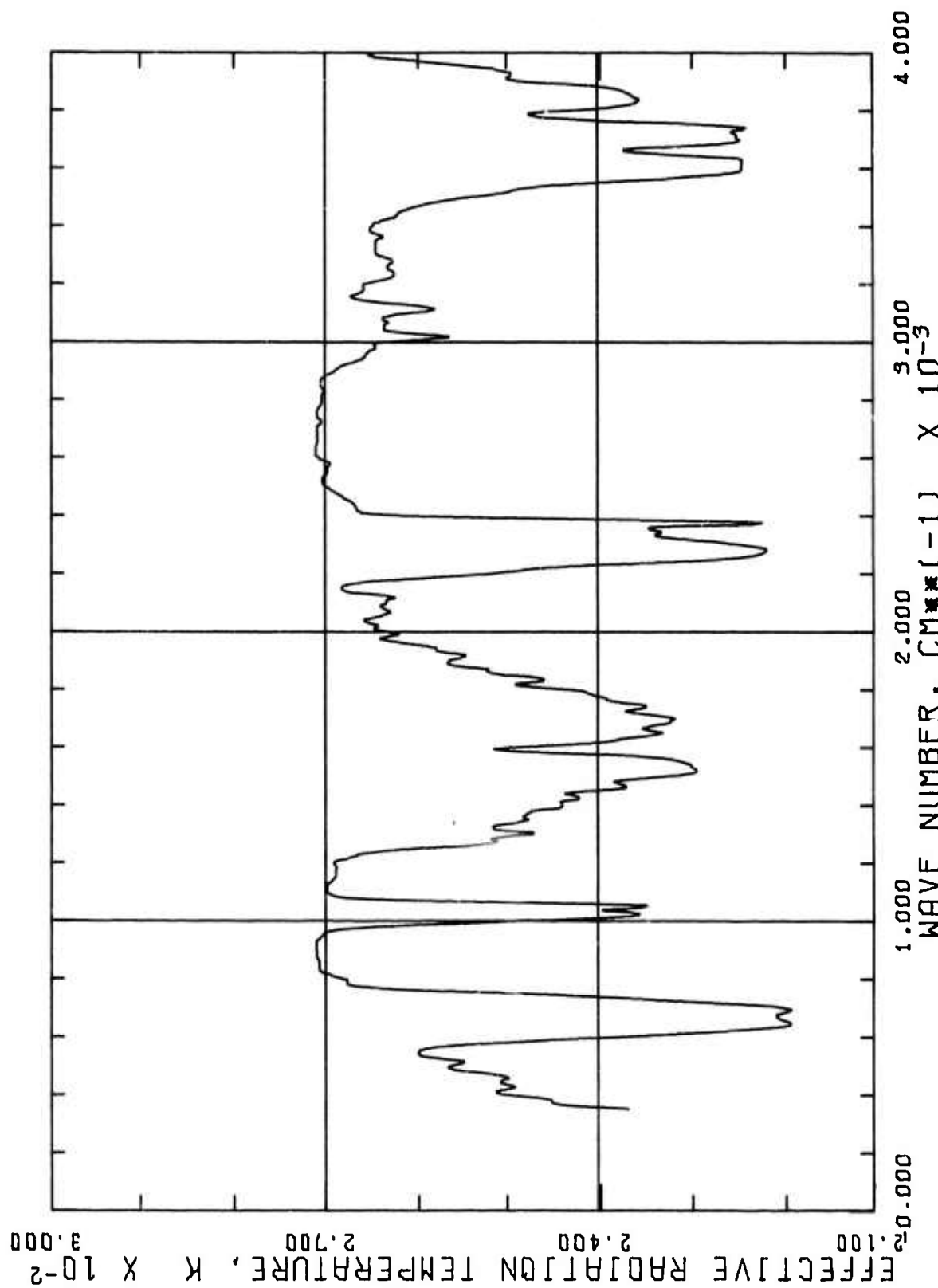
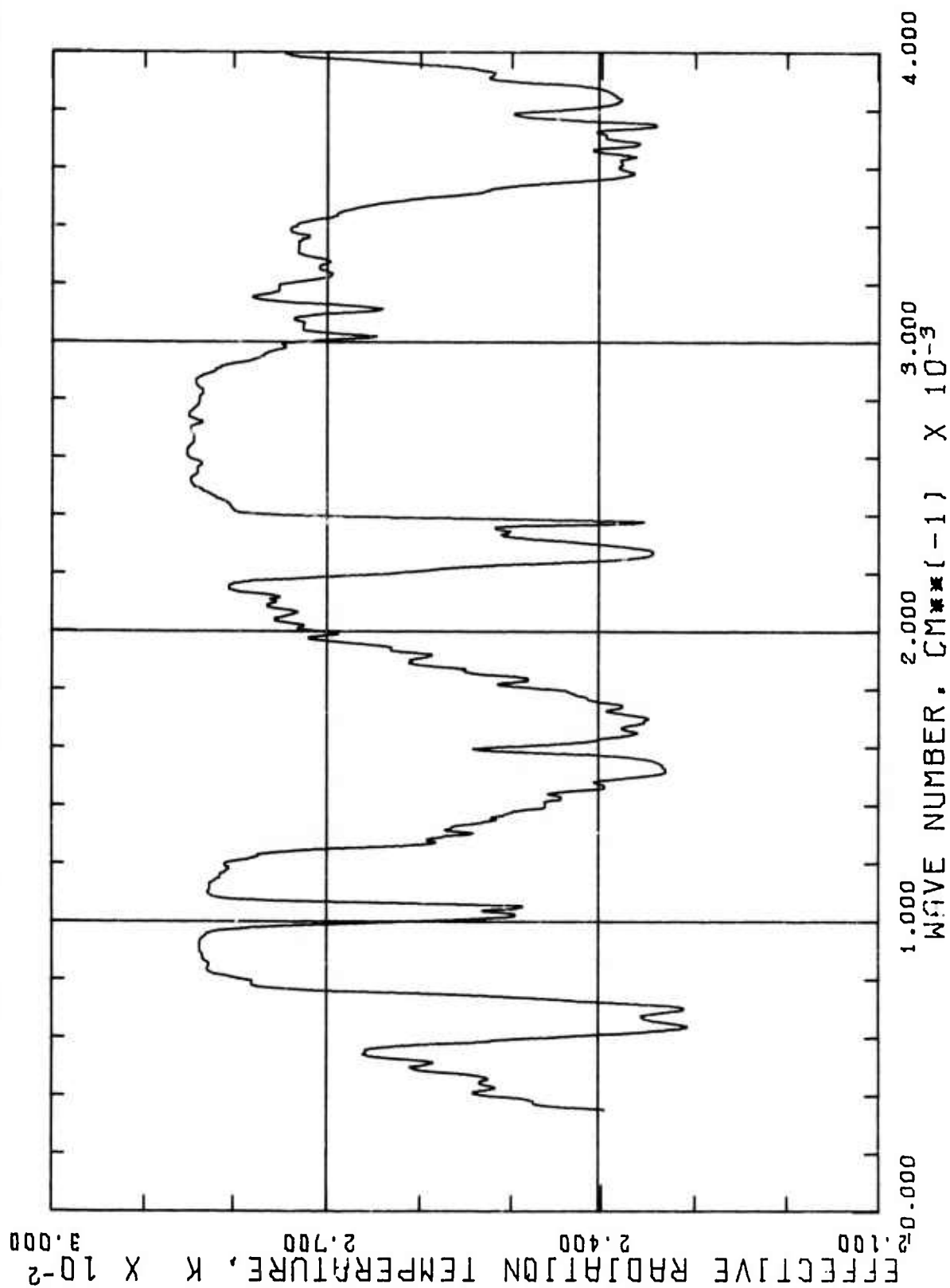
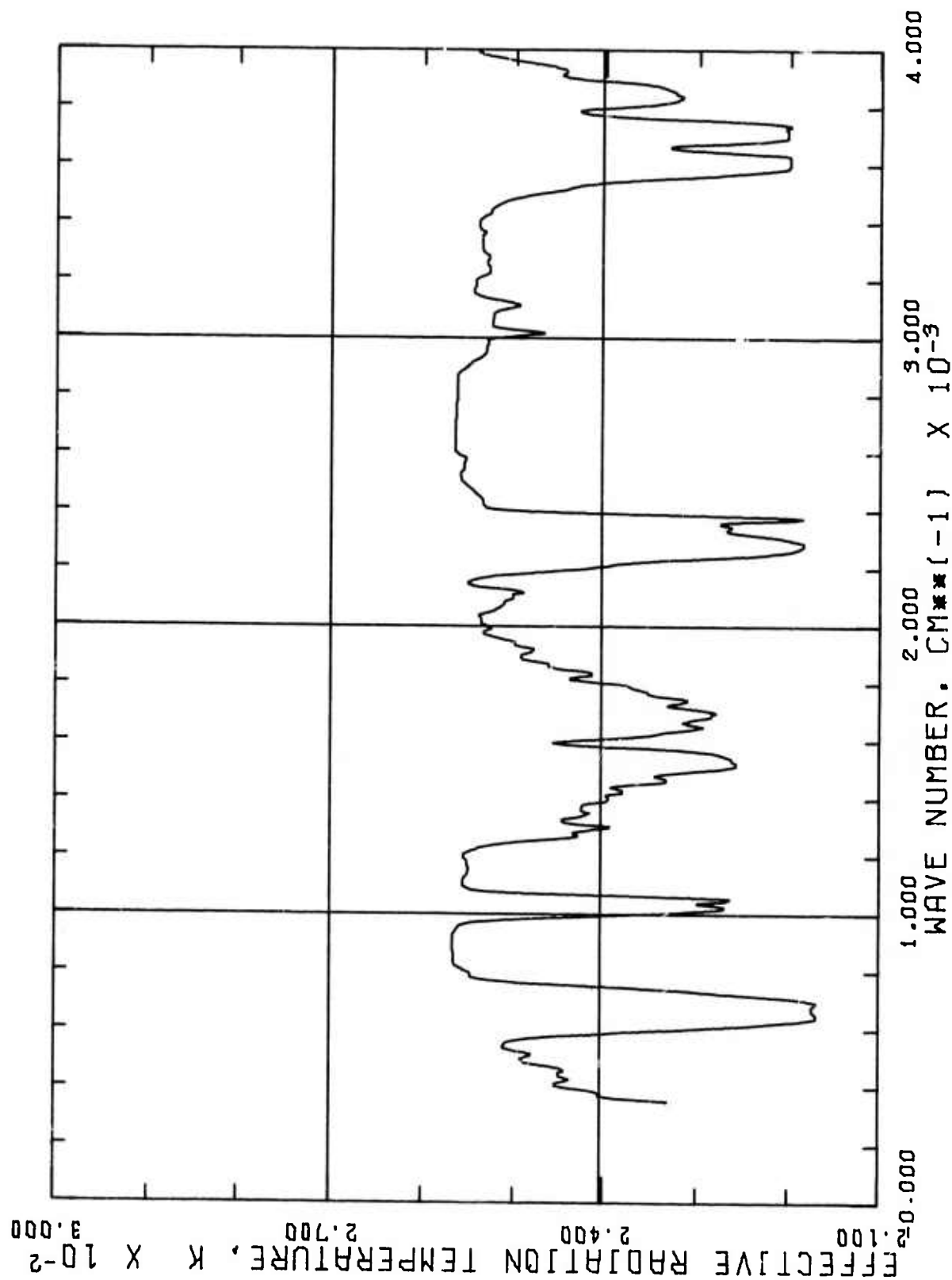


FIGURE V-3



Lower Atmosphere Radiation Temperature
For Sub-Arctic Summer Model Atmosphere

FIGURE V-4



Lower Atmosphere Radiation Temperature
For Sub-Arctic Winter Model Atmosphere

FIGURE V-5

WAVE NUMBER	MODEL				
	1	2	3	4	5
350	242.93	241.75	235.85	233.43	232.82
355	246.31	245.03	239.88	242.28	235.71
360	249.36	248.07	242.55	244.87	238.15
365	251.46	250.19	244.34	245.70	239.75
370	252.35	251.03	245.10	247.48	240.41
375	252.36	251.03	245.10	247.48	240.42
380	252.55	251.27	245.26	247.65	240.56
385	253.08	251.81	245.72	248.12	240.95
390	254.51	253.24	246.92	249.38	241.37
395	256.71	255.42	249.71	251.31	243.44
400	258.75	257.46	250.35	253.15	244.71
405	259.88	258.59	251.23	254.16	245.33
410	259.70	258.41	251.09	254.00	245.23
415	259.15	257.86	251.66	253.50	244.96
420	257.67	256.33	249.49	252.17	244.05
425	256.95	255.66	248.91	251.53	243.53
430	257.70	256.41	249.51	252.19	244.07
435	258.64	257.34	250.26	253.04	244.64
440	259.21	257.91	250.70	253.55	244.93
445	259.03	257.73	250.56	253.39	244.83
450	258.67	257.37	250.28	253.06	244.66
455	257.94	256.65	249.70	252.40	244.21
460	258.32	257.03	250.01	252.74	244.45
465	258.05	257.78	250.50	253.42	244.91
470	260.40	259.11	251.62	254.61	245.69
475	262.45	261.16	253.20	256.49	246.85
480	264.72	263.33	254.86	258.53	248.07
485	266.44	265.07	256.07	260.08	248.79
490	267.20	265.82	256.61	260.79	249.14
495	267.40	266.01	256.74	260.97	249.23
500	266.47	265.10	256.09	260.11	248.81
505	265.54	264.13	255.44	259.26	248.38
510	264.60	263.26	254.77	258.41	247.94
515	264.80	263.45	254.90	258.59	248.02
520	266.73	265.35	256.22	260.35	248.85
525	269.29	267.83	257.92	262.66	249.93
530	271.17	269.65	259.07	264.35	250.60
535	272.62	271.01	259.90	265.62	251.03
540	273.13	271.43	260.14	266.06	251.11
545	272.64	271.02	259.75	265.64	250.81
550	272.92	271.23	259.79	265.91	250.73
555	272.71	271.03	259.50	265.74	250.42
560	271.95	270.43	258.85	265.11	249.87

TABLE V-1: Effective Lower Atmosphere Radiation Temperature

WAVE NUMBER	1	MODEL 2	ATMOSPHERE		
			3	4	5
565	270.34	268.92	257.61	263.77	248.90
570	267.68	266.43	255.61	261.57	247.37
575	264.34	263.41	253.08	253.84	245.41
580	260.48	259.83	250.05	253.72	242.96
585	256.58	256.41	246.62	252.70	239.91
590	254.97	255.02	244.75	251.60	237.99
595	250.61	251.13	240.90	249.49	234.55
600	245.98	247.22	237.32	245.26	231.52
605	242.25	244.03	234.54	242.73	229.20
610	237.55	240.16	231.26	239.69	226.50
615	233.32	236.67	228.41	237.07	224.19
620	229.86	233.83	226.14	235.10	222.37
625	226.32	231.15	223.86	233.11	220.53
630	222.53	228.31	221.41	231.33	218.54
635	220.52	226.93	220.08	230.67	217.46
640	219.66	226.49	219.29	230.76	216.79
645	220.59	227.41	219.26	231.80	216.64
650	222.38	228.84	219.70	233.03	216.79
655	224.00	230.07	220.16	234.00	217.00
660	225.35	231.09	220.57	234.83	217.23
665	225.37	231.85	221.91	235.44	217.40
670	226.69	232.11	221.02	235.64	217.47
675	226.46	231.93	220.95	235.50	217.42
680	224.75	230.61	220.39	234.44	217.13
685	222.90	229.22	219.85	233.34	216.87
690	221.00	227.64	219.36	232.03	216.66
695	220.05	226.77	219.29	231.05	216.74
700	221.31	227.39	220.36	230.90	217.66
705	222.98	228.53	221.38	231.48	218.47
710	227.03	231.51	223.79	233.34	220.36
715	232.46	235.71	227.16	235.29	222.97
720	236.66	239.13	229.81	238.87	225.07
725	241.74	243.33	233.19	242.22	227.68
730	245.43	246.50	235.74	244.71	229.69
735	249.10	249.75	238.46	247.38	231.86
740	253.26	253.47	241.62	250.50	234.40
745	257.30	257.10	244.83	253.60	237.00
750	264.06	263.31	250.03	259.07	241.09
755	270.39	259.22	255.04	264.44	245.00
760	275.90	275.35	260.20	270.11	248.93
765	280.48	276.73	263.10	273.31	251.10
770	283.30	281.43	265.49	275.82	252.99
775	285.16	283.30	267.05	277.53	254.22

TABLE V-1: Continued

WAVE NUMBER	1	MODEL 2	ATMOSPHERE 3	4	5
780	285.56	283.63	267.52	277.38	254.68
785	285.71	283.81	267.54	277.99	254.83
790	285.68	283.75	267.63	277.93	254.87
795	285.80	283.86	267.71	278.03	254.93
800	285.39	284.41	269.56	278.53	255.19
805	287.56	285.43	263.75	279.58	255.58
810	288.61	286.42	263.34	280.47	255.91
815	289.39	287.12	263.74	281.14	256.13
820	290.64	288.24	271.36	282.21	256.42
825	291.11	288.64	271.58	282.59	256.53
830	291.41	288.83	271.71	282.83	256.59
835	291.46	288.91	271.72	282.84	256.61
840	291.24	288.63	271.60	282.60	256.58
845	291.18	288.61	271.54	282.52	256.56
850	291.12	288.51	271.48	282.42	256.54
855	291.36	288.72	271.57	282.62	256.57
860	291.70	289.01	271.70	282.88	256.61
865	292.11	289.33	271.85	283.21	256.67
870	292.42	289.61	271.96	283.45	256.71
875	292.46	289.62	271.95	283.46	256.70
880	292.45	289.61	271.94	283.43	256.69
885	292.54	289.65	271.95	283.48	256.70
890	292.75	289.77	271.90	283.58	256.71
895	292.84	289.87	271.03	283.68	256.72
900	292.93	289.93	271.07	283.77	256.73
905	292.92	289.91	271.00	283.68	256.69
910	292.91	289.87	271.95	283.65	256.66
915	292.88	289.83	271.89	283.59	256.61
920	292.90	289.81	271.84	283.57	256.56
925	293.15	289.93	271.85	283.74	256.51
930	293.07	289.83	271.72	283.63	256.41
935	292.96	289.75	271.56	283.49	256.23
940	292.79	289.57	271.41	283.32	256.18
945	292.54	289.33	271.24	283.17	256.07
950	292.39	289.12	271.07	282.86	255.94
955	292.25	288.93	263.94	282.71	255.81
960	292.16	288.81	263.75	282.53	255.65
965	291.85	288.33	263.22	282.02	255.12
970	291.24	287.54	263.40	281.22	254.34
975	289.56	285.13	263.93	278.82	251.93
980	288.49	283.63	264.32	277.30	250.44
985	286.03	280.44	261.01	274.18	247.29
990	282.45	275.73	256.20	269.61	242.83

TABLE V-1: Continued

WAVE NUMBER	MODEL				
	1	2	3	4	5
995	279.31	271.83	252.53	265.92	239.64
1000	275.50	267.53	243.45	261.90	236.29
1005	269.61	261.23	242.92	255.39	232.07
1010	265.15	257.04	237.56	253.03	229.73
1015	259.98	253.02	236.47	251.07	227.56
1020	258.34	251.91	235.57	249.32	226.86
1025	258.60	252.03	235.71	249.42	226.97
1030	261.33	253.93	237.16	250.75	228.07
1035	265.48	257.32	239.73	253.22	229.84
1040	264.85	256.75	239.29	252.77	229.52
1045	258.30	251.85	235.48	249.24	226.30
1050	256.93	250.90	234.75	248.64	226.28
1055	257.68	251.43	235.18	249.06	226.53
1060	270.03	261.77	243.42	256.75	232.47
1065	278.40	271.12	252.01	265.14	239.33
1070	285.56	281.25	261.98	274.31	248.42
1075	289.95	285.47	266.13	279.04	252.26
1080	291.69	287.62	268.18	281.19	254.13
1085	292.52	288.56	269.06	282.11	254.92
1090	292.82	288.83	269.41	282.44	255.24
1095	293.59	289.21	269.77	282.75	255.56
1100	292.93	289.03	269.80	282.65	255.64
1105	292.72	288.91	269.75	282.48	255.64
1110	292.61	288.73	269.67	282.37	255.57
1115	292.78	288.93	269.69	282.47	255.53
1120	292.87	288.91	269.58	282.47	255.36
1125	293.01	288.53	269.52	282.51	255.25
1130	293.07	288.99	269.45	282.52	255.15
1135	292.65	288.63	269.19	282.14	254.93
1140	292.29	288.33	268.99	281.86	254.88
1145	292.00	288.07	268.87	281.66	254.83
1150	291.56	287.71	268.66	281.31	254.75
1155	291.49	287.71	268.75	281.33	254.90
1160	291.31	287.64	268.84	281.27	255.06
1165	290.89	287.37	268.82	281.04	255.16
1170	290.37	287.00	268.73	280.70	255.21
1175	290.04	286.75	268.66	280.49	255.24
1180	289.81	286.53	268.59	280.33	255.24
1185	289.78	286.53	268.58	280.33	255.26
1190	290.32	287.07	268.91	280.90	255.46
1195	290.53	287.26	269.05	281.39	255.56
1200	290.20	287.01	268.94	280.74	255.54
1205	289.48	286.41	268.65	280.20	255.42

TABLE V-1: Continued

WAVE NUMBER	1	2	3	4	5
1210	288.40	285.47	263.12	273.30	255.14
1215	287.04	284.23	267.44	273.17	254.70
1220	286.40	283.63	265.27	277.61	254.44
1225	285.92	283.20	265.44	277.14	253.98
1230	285.87	283.03	265.13	277.02	253.64
1235	284.81	282.15	265.26	275.14	252.73
1240	283.11	280.43	264.01	274.58	252.04
1245	281.53	278.13	262.21	272.32	250.77
1250	277.40	275.31	260.21	267.69	249.41
1255	272.12	270.33	255.80	265.07	247.15
1260	268.84	267.31	254.27	262.21	245.16
1265	265.60	264.20	252.01	259.44	243.56
1270	264.07	262.87	250.89	258.13	242.70
1275	264.65	263.40	251.20	258.61	243.01
1280	265.40	264.13	251.80	258.31	243.45
1285	264.83	263.54	251.16	258.73	242.78
1290	263.36	262.12	249.69	257.45	241.45
1295	262.63	261.41	248.93	256.92	240.75
1300	261.00	260.97	245.87	254.64	237.10
1305	259.32	258.30	246.91	254.09	236.28
1310	262.28	261.19	247.90	255.54	242.16
1315	263.20	262.03	251.42	257.33	243.84
1320	262.33	261.23	251.50	256.48	244.52
1325	262.19	261.07	251.66	256.32	244.72
1330	261.62	260.54	251.85	255.94	244.15
1335	259.69	258.70	249.51	254.18	242.89
1340	258.56	257.61	248.68	253.19	242.27
1345	257.86	256.94	248.00	252.59	241.77
1350	256.70	255.73	247.30	251.54	241.34
1355	257.44	256.45	249.13	252.12	242.11
1360	257.21	256.15	248.25	251.81	242.44
1365	256.19	255.05	247.74	250.78	242.30
1370	255.72	254.53	247.50	250.31	242.23
1375	255.19	253.95	247.19	249.78	242.10
1380	254.98	253.70	247.10	249.55	242.10
1385	253.66	252.34	246.05	248.36	241.26
1390	251.30	249.95	244.08	246.23	239.55
1395	251.02	249.65	243.85	245.97	239.34
1400	251.05	249.63	243.87	245.00	239.38
1405	251.24	249.67	244.03	245.17	239.53
1410	251.43	250.07	244.20	245.33	239.67
1415	250.74	249.37	243.60	245.72	239.14
1420	249.02	247.63	242.10	244.22	237.78

TABLE V-1: Continued

Reproduced from
best available copy.

WAVE NUMBER	1	MODEL 2	ATMOSPHERE			5
			3	4		
1425	242.03	247.64	242.00	244.21	237.77	
1430	249.34	247.95	242.36	244.49	238.02	
1435	250.16	243.80	243.08	243.22	238.56	
1440	250.85	249.43	243.57	245.82	239.13	
1445	249.48	248.11	242.48	244.62	238.12	
1450	247.50	246.03	240.72	242.86	236.49	
1455	245.08	243.63	233.53	240.72	234.41	
1460	243.49	242.04	237.07	239.77	233.03	
1465	243.51	242.05	237.08	239.38	233.04	
1470	244.01	242.54	237.54	239.79	233.47	
1475	244.51	243.04	237.99	240.22	233.91	
1480	245.01	243.54	238.45	240.64	234.35	
1485	244.23	242.75	237.74	239.97	233.67	
1490	242.36	240.83	235.01	238.40	232.01	
1495	241.02	239.56	234.75	237.28	230.77	
1500	239.12	237.60	232.96	235.74	229.01	
1505	237.13	235.81	231.09	234.22	227.22	
1510	235.31	234.67	229.93	233.36	226.13	
1515	235.40	234.10	229.44	232.99	225.65	
1520	235.27	234.07	229.31	232.91	225.53	
1525	235.53	234.31	229.55	233.18	225.76	
1530	236.03	234.70	230.04	233.44	226.23	
1535	236.14	234.80	230.15	233.52	226.33	
1540	236.14	234.84	230.15	233.52	226.33	
1545	236.58	235.23	230.55	233.82	226.71	
1550	237.17	235.83	231.10	234.24	227.23	
1555	237.62	236.23	231.52	234.57	227.64	
1560	238.52	237.09	232.37	235.24	228.43	
1565	240.29	238.82	234.04	236.64	230.05	
1570	242.40	240.91	236.03	238.39	232.02	
1575	245.90	244.44	239.26	241.40	235.11	
1580	250.78	249.41	243.61	245.72	239.16	
1585	255.80	254.43	247.34	250.21	242.80	
1590	259.29	258.00	250.64	253.36	245.02	
1595	260.41	259.13	251.51	254.38	245.67	
1600	257.81	256.51	249.46	252.02	244.10	
1605	257.62	252.23	246.02	248.25	241.25	
1610	250.26	248.83	243.15	245.27	238.73	
1615	247.90	246.43	241.05	243.15	236.80	
1620	245.77	244.31	239.13	241.27	234.98	
1625	244.65	243.17	238.10	240.29	234.01	
1630	244.03	242.55	237.53	239.76	233.47	
1635	242.35	240.85	235.97	238.32	231.95	

TABLE V-1: Continued

WAVE NUMBER	1	MODEL 2	ATMOSPHERE 3	4	5
1640	241.16	235.67	234.84	237.32	230.86
1645	240.80	238.51	233.74	236.37	229.77
1653	239.43	237.95	233.24	235.92	229.25
1655	240.03	238.54	233.77	236.39	229.83
1660	241.23	239.73	234.61	237.37	230.92
1665	241.69	240.13	235.34	237.76	231.35
1670	241.10	239.63	234.78	237.26	230.80
1675	240.52	239.11	234.23	236.78	230.24
1680	239.44	238.01	233.25	235.75	229.23
1685	238.40	237.01	232.23	235.15	228.35
1690	238.48	237.00	232.27	235.15	228.34
1695	237.19	236.72	231.90	234.92	226.83
1700	237.90	236.45	231.71	234.71	227.81
1705	237.77	237.21	232.53	235.36	228.57
1710	240.23	238.73	233.90	236.51	229.93
1715	241.42	239.83	235.02	237.50	231.00
1720	242.81	241.27	236.37	238.66	232.37
1725	243.75	242.24	237.23	239.48	233.13
1730	242.99	241.45	236.51	238.91	232.48
1735	241.91	240.35	235.45	237.89	231.44
1740	241.42	239.85	234.94	237.47	230.92
1745	241.34	239.03	234.93	237.41	230.92
1750	242.45	240.51	235.02	238.36	232.01
1755	244.35	242.85	237.81	239.98	233.74
1760	245.17	243.67	238.55	240.69	234.45
1765	246.00	244.51	239.32	241.41	235.17
1770	246.18	244.63	239.47	241.56	235.31
1775	246.52	245.04	239.78	241.87	235.61
1780	247.36	245.90	240.55	242.61	236.33
1785	247.87	246.42	241.03	243.06	236.77
1790	248.38	246.95	241.47	243.53	237.20
1795	248.73	247.33	241.70	243.84	237.43
1800	250.10	248.71	242.90	245.06	238.61
1805	252.94	251.53	245.43	247.58	240.77
1810	255.48	254.15	247.54	249.97	242.57
1815	257.32	256.01	249.05	251.53	243.73
1820	257.15	255.84	248.90	251.37	243.68
1825	255.15	253.82	247.27	249.57	242.34
1830	253.36	251.93	245.70	247.94	241.06
1835	253.37	252.02	245.75	247.96	241.08
1840	253.93	252.53	246.26	248.46	241.49
1845	255.39	254.07	247.48	249.79	242.52
1850	259.09	257.81	251.45	253.14	244.91

TABLE V-1: Continued

Reproduced from
best available copy.

WAVE NUMBER	1	MODEL 2	ATMOSPHERE		
			3	4	5
1855	260.41	259.12	251.50	254.34	245.69
1860	261.17	259.83	252.04	255.04	246.13
1865	261.56	260.23	252.34	255.39	246.35
1870	261.01	259.73	251.96	254.89	246.04
1875	263.47	262.17	253.80	257.14	247.37
1880	265.34	264.04	255.15	258.87	248.28
1885	267.18	265.85	256.42	260.57	249.11
1890	267.35	265.51	256.84	261.17	249.35
1895	267.35	266.02	256.46	261.72	249.07
1900	267.88	266.51	256.73	261.19	249.17
1905	266.93	265.61	256.73	261.32	248.67
1910	265.69	264.33	255.13	259.18	248.04
1915	265.10	263.81	254.70	258.64	247.75
1920	264.95	263.65	254.59	258.50	247.68
1925	267.01	265.67	255.02	261.39	248.62
1930	269.12	267.71	257.43	262.31	249.51
1935	270.07	268.64	258.12	263.19	249.89
1940	270.10	268.67	258.20	263.22	250.11
1945	269.68	268.27	257.93	262.84	250.01
1950	271.30	269.83	259.05	264.32	250.69
1955	272.70	271.15	259.56	265.59	251.25
1960	274.88	273.13	261.23	267.52	251.99
1965	276.99	275.13	262.41	269.35	252.61
1970	278.88	276.83	263.41	271.97	253.15
1975	279.91	277.74	263.95	271.85	253.44
1980	279.47	277.35	263.74	271.48	253.34
1985	278.02	276.07	263.00	271.24	252.96
1990	275.14	274.35	261.99	269.63	252.42
1995	276.68	274.85	262.28	269.09	252.57
2000	275.90	276.85	263.45	271.98	253.13
2005	280.37	278.14	264.18	272.21	253.55
2010	281.62	279.22	264.77	273.23	253.84
2015	280.80	278.57	264.35	272.55	253.51
2020	280.41	278.15	264.12	272.22	253.46
2025	281.69	279.25	264.63	273.24	253.69
2030	283.25	280.55	265.31	274.47	253.91
2035	284.53	281.53	265.71	275.41	253.93
2040	284.95	281.84	265.61	275.63	253.74
2045	284.64	281.44	265.05	275.24	253.18
2050	283.80	280.57	264.19	274.39	252.41
2055	283.41	280.15	263.79	273.98	252.07
2060	282.87	279.65	263.42	273.48	251.79
2065	282.31	279.07	262.97	272.93	251.40

TABLE V-1: Continued

WAVE NUMBER	1	MODEL 2	ATMOSPHERE 3	4	5
2070	283.40	279.83	263.14	273.57	251.23
2075	284.59	280.62	263.33	274.26	251.07
2080	285.91	282.22	263.78	275.67	250.93
2085	288.04	282.97	264.03	275.33	250.91
2090	288.28	282.95	263.83	275.28	250.53
2095	287.54	282.52	263.42	275.32	250.13
2100	287.32	282.05	263.23	275.38	251.04
2105	287.46	282.11	263.19	275.43	249.96
2110	286.14	282.65	263.47	275.92	250.10
2115	287.61	281.71	262.22	274.93	248.31
2120	287.56	281.91	262.70	275.16	249.32
2125	288.05	282.61	263.51	275.38	250.17
2130	289.23	284.15	263.20	277.47	251.89
2135	290.55	286.03	267.33	273.42	254.05
2140	291.61	286.33	267.74	273.78	254.56
2145	291.67	286.83	269.22	281.34	255.04
2150	291.23	286.93	269.21	281.43	255.03
2155	291.34	286.93	267.99	281.39	254.70
2160	291.24	286.75	267.57	281.14	254.30
2165	291.07	286.33	266.92	279.73	253.74
2170	289.88	285.22	265.83	273.58	252.88
2175	288.44	283.84	264.61	277.24	251.94
2180	285.07	280.68	261.95	274.21	249.33
2185	281.82	277.65	259.41	271.31	247.69
2190	278.90	274.91	257.10	263.71	246.06
2195	274.82	271.11	253.92	265.14	243.52
2200	272.04	268.55	251.81	262.75	241.36
2205	270.15	266.85	250.44	261.17	240.73
2210	267.45	264.33	248.43	259.91	239.22
2215	266.63	263.61	247.78	258.20	238.71
2220	264.19	261.35	245.80	256.15	237.13
2225	261.02	258.43	243.44	253.53	235.23
2230	257.53	255.23	240.87	251.76	233.17
2235	252.01	250.38	236.92	246.56	230.07
2240	246.89	245.93	233.44	242.94	227.32
2245	240.37	240.51	229.17	238.90	224.01
2250	236.70	237.53	225.85	235.95	222.22
2255	234.26	235.77	225.44	235.85	221.08
2260	231.20	233.62	223.74	234.75	219.76
2265	229.63	232.63	222.90	234.38	219.12
2270	228.59	232.05	222.37	234.28	218.71
2275	227.81	231.71	221.97	234.37	218.33
2280	227.39	231.67	221.79	234.73	218.19

TABLE V-1: Continued

WAVE NUMBER	1	MODEL 2	ATMOSPHERE 3	4	5
2285	227.60	232.13	221.96	235.54	218.22
2290	228.60	233.32	222.46	235.73	218.49
2295	230.08	234.75	223.25	238.11	218.94
2300	232.16	236.67	224.46	239.86	219.67
2305	234.51	238.89	225.73	241.90	220.63
2310	236.22	240.43	227.10	243.39	221.43
2315	238.60	242.63	228.94	245.46	222.79
2320	240.95	245.03	230.87	247.77	224.35
2325	243.07	247.09	232.83	249.80	225.82
2330	244.05	248.17	233.98	250.93	226.71
2335	244.27	248.41	234.11	251.17	226.90
2340	243.51	247.55	233.20	250.30	226.21
2345	243.33	247.35	233.11	250.08	226.04
2350	244.21	248.35	234.06	251.11	226.86
2355	244.85	249.02	234.70	251.78	227.38
2360	244.97	249.14	234.81	251.89	227.49
2365	242.00	246.03	231.81	248.82	225.09
2370	231.24	235.83	223.94	239.11	219.34
2375	228.05	232.59	222.18	235.89	218.34
2380	232.30	234.35	224.10	235.18	220.05
2385	248.38	247.55	234.06	243.70	227.72
2390	262.73	259.73	244.15	254.54	235.74
2395	274.62	270.67	253.06	264.53	242.88
2400	284.50	279.85	260.62	273.18	248.95
2405	289.28	284.29	264.27	277.41	251.81
2410	291.64	286.43	266.06	279.52	253.21
2415	291.94	286.75	266.28	279.78	253.36
2420	292.21	286.99	266.48	280.02	253.49
2425	292.32	287.07	266.56	280.13	253.54
2430	292.44	287.21	266.65	280.24	253.59
2435	292.62	287.35	266.77	280.39	253.66
2440	292.74	287.45	266.85	280.50	253.70
2445	292.98	287.67	267.02	280.71	253.82
2450	293.30	287.95	267.26	280.99	253.97
2455	293.74	288.37	267.50	281.39	254.19
2460	294.16	288.75	267.90	281.77	254.40
2465	294.43	288.99	268.10	282.01	254.53
2470	294.77	289.30	268.35	282.31	254.69
2475	295.10	289.60	268.50	282.61	254.84
2480	295.44	289.90	268.84	282.91	255.00
2485	295.88	290.30	269.17	283.31	255.22
2490	296.22	290.61	269.42	283.61	255.40
2495	296.54	290.91	269.66	283.90	255.57

TABLE V-1: Continued

WAVE NUMBER	1	MODEL 2	ATMOSPHERE 3	4	5
2510	296.91	291.24	269.94	284.24	255.75
2535	297.24	291.55	270.13	284.54	255.91
2510	297.33	291.63	270.26	284.62	255.95
2515	297.46	291.75	270.36	284.74	256.02
2520	297.50	291.78	270.40	284.78	256.03
2525	297.39	291.63	270.32	284.69	255.97
2530	297.15	291.47	270.16	284.49	255.84
2535	296.87	291.21	269.96	284.24	255.69
2540	296.57	290.94	269.75	283.99	255.52
2545	296.35	290.74	269.60	283.80	255.39
2550	296.24	290.65	269.55	283.72	255.36
2555	296.27	290.71	269.60	283.77	255.40
2560	296.31	290.75	269.67	283.82	255.46
2565	296.19	290.66	269.63	283.75	255.44
2570	295.82	290.42	269.45	283.51	255.30
2575	295.66	290.23	269.30	283.31	255.20
2580	295.67	290.23	269.36	283.35	255.26
2585	296.06	290.62	269.71	283.73	255.52
2590	296.55	291.03	270.14	284.19	255.87
2595	297.02	291.54	270.54	284.63	256.13
2600	297.32	291.82	270.78	284.91	256.36
2605	297.53	292.03	270.99	285.12	256.52
2610	297.56	292.03	271.07	285.18	256.59
2615	297.57	292.13	271.09	285.19	256.61
2620	297.38	291.95	271.04	285.16	256.60
2625	297.25	291.85	270.99	284.97	256.59
2630	297.16	291.73	270.95	284.91	256.56
2635	296.92	291.61	270.87	284.74	256.53
2640	296.70	291.44	270.80	284.59	256.50
2645	296.52	291.33	270.73	284.47	256.49
2650	296.19	291.05	270.62	284.24	256.43
2655	296.13	291.01	270.60	284.20	256.43
2660	296.10	290.93	270.59	284.18	256.43
2665	296.15	291.02	270.62	284.21	256.44
2670	296.39	291.21	270.70	284.38	256.47
2675	296.44	291.24	270.72	284.42	256.48
2680	296.56	291.35	270.77	284.52	256.50
2685	296.70	291.51	270.85	284.66	256.54
2690	296.81	291.54	270.87	284.69	256.55
2695	296.91	291.62	270.91	284.76	256.57
2700	296.96	291.65	270.93	284.78	256.57
2705	296.61	291.34	270.80	284.55	256.52
2710	296.04	290.95	270.61	284.16	256.44

TABLE V-1: Continued

WAVE NUMBER	1	MODEL 2	ATMOSPHERE 3	4	5
2715	295.35	290.44	270.37	283.69	256.34
2720	294.80	290.03	270.18	283.32	256.26
2725	295.06	290.22	270.26	283.48	256.29
2730	295.95	290.83	270.56	284.08	256.41
2735	296.68	291.41	270.79	284.56	256.49
2740	297.14	291.76	270.94	284.88	256.54
2745	297.20	291.80	270.95	284.92	256.54
2750	297.01	291.65	270.88	284.77	256.50
2755	296.80	291.47	270.80	284.63	256.47
2760	296.58	291.32	270.72	284.48	256.43
2765	296.32	291.12	270.61	284.29	256.37
2770	296.05	290.90	270.50	284.03	256.31
2775	295.79	290.70	270.38	283.90	256.25
2780	295.55	290.51	270.27	283.72	256.18
2785	295.37	290.36	270.19	283.59	256.15
2790	295.24	290.27	270.16	283.51	256.14
2795	295.29	290.31	270.18	283.55	256.15
2800	295.29	290.34	270.23	283.59	256.21
2805	295.27	290.34	270.25	283.59	256.24
2810	295.17	290.27	270.23	283.53	256.25
2815	295.01	290.15	270.17	283.42	256.23
2820	294.63	289.87	270.03	283.16	256.16
2825	294.67	289.89	270.04	283.18	256.16
2830	294.75	289.96	270.07	283.24	256.18
2835	294.97	290.13	270.16	283.40	256.22
2840	295.37	290.43	270.30	283.68	256.29
2845	295.73	290.74	270.46	283.95	256.36
2850	296.02	290.91	270.53	284.11	256.39
2855	296.20	291.03	270.55	284.21	256.37
2860	296.17	290.90	270.51	284.17	256.33
2865	296.12	290.94	270.45	284.12	256.28
2870	295.95	290.80	270.34	283.98	256.21
2875	295.60	290.43	270.12	283.68	256.06
2880	295.20	290.15	269.86	283.36	255.90
2885	294.85	289.85	269.56	283.08	255.74
2890	294.24	289.32	269.30	282.59	255.51
2895	293.48	288.71	268.92	282.01	255.27
2900	293.29	288.51	268.73	281.81	255.11
2905	293.19	288.37	268.54	281.67	254.94
2910	292.79	288.00	268.26	281.32	254.72
2915	292.45	287.71	268.06	281.05	254.59
2920	291.85	287.23	267.75	280.59	254.40
2925	290.81	286.37	267.25	279.80	254.09

TABLE V-1: Continued

WAVE NUMBER	MODEL				
	1	2	3	4	5
2930	289.24	285.12	266.57	273.64	253.73
2935	288.37	284.42	265.21	272.98	253.55
2940	287.69	283.84	265.36	272.43	253.33
2945	287.06	283.32	265.55	275.95	253.16
2950	286.59	282.93	265.35	275.58	253.05
2955	286.47	282.84	265.32	275.50	253.05
2960	286.12	282.57	265.22	275.24	253.03
2965	285.74	282.27	265.19	275.96	253.01
2970	284.95	281.65	264.87	275.40	252.98
2975	283.93	280.84	264.52	274.64	252.87
2980	283.40	280.42	264.35	274.26	252.84
2985	283.75	280.75	264.62	274.58	253.02
2990	283.94	280.91	264.74	274.71	253.11
2995	284.10	281.02	264.76	274.81	253.11
3000	282.34	279.31	263.37	273.15	251.92
3005	279.33	275.45	261.89	270.38	250.05
3010	276.80	274.11	259.57	268.12	248.65
3015	273.11	270.63	255.39	264.86	246.66
3020	272.65	270.37	255.53	264.59	246.97
3025	275.14	272.85	253.90	265.29	249.11
3030	277.61	275.23	261.21	269.35	250.34
3035	279.50	277.02	262.48	271.01	251.83
3040	281.25	278.61	263.58	272.53	252.56
3045	281.25	278.57	263.50	272.50	252.48
3050	281.41	278.61	263.48	272.59	252.40
3055	281.30	278.64	263.46	272.56	252.44
3060	281.16	278.53	263.39	272.48	252.40
3065	281.75	278.13	263.17	272.15	252.23
3070	281.49	278.81	263.43	272.72	252.36
3075	282.49	279.62	263.82	273.50	252.51
3080	282.40	279.53	263.70	273.40	252.40
3085	281.92	279.11	263.44	273.01	252.24
3090	281.44	277.85	262.74	271.82	251.90
3095	278.91	276.55	262.02	270.60	251.54
3100	276.62	274.55	261.92	268.70	250.99
3105	272.91	271.24	259.01	265.54	250.00
3110	271.34	269.79	258.15	264.15	249.55
3115	271.07	269.54	258.02	263.91	249.43
3120	272.67	271.04	259.57	265.35	250.13
3125	274.63	272.84	260.15	267.07	250.79
3130	277.70	275.60	261.83	269.71	251.72
3135	281.52	278.91	263.73	272.85	252.72
3140	284.47	281.43	265.20	275.23	253.51

TABLE V-1: Continued

WAVE NUMBER	1	MODEL 2	ATMOSPHERE 3	4	5
3145	286.52	283.17	265.21	275.88	254.37
3150	287.44	283.93	265.77	277.66	254.43
3155	287.78	284.31	267.06	277.98	254.56
3160	287.00	283.72	266.87	277.43	254.68
3165	285.35	282.33	265.24	275.14	254.45
3170	284.48	281.63	265.94	275.53	254.37
3175	283.70	281.04	265.61	274.93	254.24
3180	283.63	280.93	265.61	274.88	254.25
3185	283.59	281.05	265.67	274.95	254.31
3190	283.74	281.11	265.72	275.00	254.35
3195	283.91	281.25	265.81	275.15	254.40
3200	283.37	280.73	265.56	274.71	254.33
3205	281.90	279.54	264.89	273.53	253.98
3210	280.51	278.34	264.22	272.38	253.65
3215	278.90	276.91	263.40	271.03	253.24
3220	279.07	276.13	262.97	271.32	253.01
3225	277.23	275.42	262.53	269.59	252.78
3230	276.90	275.12	262.35	269.30	252.68
3235	276.90	275.12	262.35	269.31	252.69
3240	277.43	275.61	262.63	269.77	252.84
3245	277.77	275.92	262.82	270.07	252.93
3250	278.63	276.68	263.26	270.81	253.17
3255	278.64	276.67	263.27	270.81	253.17
3260	278.48	276.55	263.18	270.68	253.13
3265	278.15	276.26	263.01	270.40	253.04
3270	277.48	275.65	262.66	269.82	252.85
3275	277.15	275.35	262.48	269.53	252.76
3280	277.67	275.82	262.76	269.98	252.91
3285	277.85	275.93	262.86	270.14	252.96
3290	279.20	277.13	263.55	271.29	253.31
3295	280.16	278.04	264.03	272.09	253.55
3300	280.79	278.53	264.33	272.60	253.69
3305	281.23	278.95	264.53	272.87	253.78
3310	281.22	278.95	264.52	272.96	253.77
3315	281.07	278.81	264.44	272.83	253.73
3320	281.09	278.83	264.45	272.85	253.74
3325	280.96	278.73	264.45	272.75	253.72
3330	281.14	278.83	264.50	272.90	253.77
3335	281.15	278.89	264.49	272.90	253.77
3340	281.13	278.87	264.47	272.88	253.75
3345	281.09	278.83	264.44	272.85	253.72
3350	280.73	278.51	264.23	272.53	253.60
3355	280.52	278.32	264.10	272.35	253.52

TABLE V-1: Continued

WAVE NUMBER	1	MODEL 2	ATMOSPHERE		
			3	4	5
3360	272.71	277.61	263.66	271.67	253.31
3365	272.75	277.65	263.72	271.71	253.33
3370	280.78	278.55	264.26	272.58	253.62
3375	281.63	279.31	264.70	273.29	253.86
3380	282.27	279.85	265.02	273.83	254.03
3385	282.48	280.05	265.14	274.01	254.11
3390	282.21	279.82	265.03	273.80	254.06
3395	281.95	279.57	264.90	273.56	253.93
3400	281.32	279.03	264.61	273.06	253.85
3405	281.33	279.05	264.61	273.07	253.85
3410	280.87	278.65	264.39	272.69	253.74
3415	280.08	277.97	264.00	272.03	253.54
3420	279.27	277.25	263.59	271.36	253.34
3425	278.28	276.33	263.07	270.51	253.08
3430	276.93	275.15	262.36	269.34	252.71
3435	276.41	274.63	262.08	268.89	252.55
3440	276.25	274.54	261.99	268.74	252.50
3445	276.07	274.33	261.89	268.59	252.44
3450	275.71	274.05	261.68	268.27	252.33
3455	275.17	273.55	261.36	267.79	252.14
3460	274.23	272.67	260.80	266.94	251.81
3465	273.63	272.03	260.41	266.38	251.57
3470	272.64	271.15	259.76	265.47	251.13
3475	271.97	270.51	259.32	264.86	250.88
3480	271.07	269.64	258.68	264.01	250.45
3485	269.39	268.03	257.54	262.46	249.71
3490	268.11	266.77	256.56	261.24	248.98
3495	266.63	265.31	255.44	259.85	248.16
3500	265.37	264.07	254.47	258.68	247.44
3505	262.66	261.43	252.44	256.16	245.98
3510	261.35	260.13	251.36	254.94	245.12
3515	259.79	258.55	250.12	253.51	244.16
3520	259.07	257.84	249.52	252.85	243.67
3525	258.60	257.37	248.96	252.41	243.03
3530	257.93	256.71	248.19	251.77	242.31
3535	256.86	255.65	246.96	250.79	241.07
3540	255.30	254.13	245.46	249.41	239.67
3545	252.47	251.33	242.94	246.98	237.43
3550	249.64	248.65	240.47	244.65	235.24
3555	246.44	245.61	237.62	242.15	232.63
3560	243.69	243.11	235.14	240.25	230.29
3565	240.75	240.52	232.36	238.48	227.64
3570	239.01	239.07	231.75	237.56	226.07

TABLE V-1: Continued

WAVE NUMBER	1	MODEL 2	ATMOSPHERE		
			3	4	5
3575	236.62	237.27	229.54	235.75	223.95
3580	234.62	235.94	226.64	235.36	222.25
3585	232.96	235.17	225.29	235.46	220.78
3590	232.04	235.02	224.54	237.16	219.98
3595	231.92	235.31	224.43	237.76	219.81
3600	231.98	235.51	224.48	239.08	219.79
3605	231.89	235.35	224.42	237.86	219.84
3610	231.81	235.14	224.39	237.57	219.87
3615	231.75	235.11	224.34	237.58	219.89
3620	231.83	235.23	224.38	237.83	219.88
3625	231.93	235.44	224.45	238.01	219.86
3630	231.91	235.23	224.46	237.58	219.92
3635	232.59	234.93	225.03	235.54	220.57
3640	235.61	236.35	227.94	235.17	223.56
3645	238.91	238.71	231.17	237.15	226.74
3650	241.59	240.93	233.97	238.39	229.53
3655	243.84	242.83	235.21	239.83	231.77
3660	245.10	244.07	237.40	240.76	232.93
3665	245.05	244.02	237.34	240.72	232.87
3670	243.16	242.27	235.51	239.38	231.09
3675	239.87	239.35	232.34	237.37	227.99
3680	235.47	236.62	229.06	235.92	224.82
3685	233.83	235.05	226.50	235.67	222.27
3690	232.78	234.89	225.27	235.32	220.91
3695	232.08	235.21	224.59	237.51	220.36
3700	232.54	236.27	224.91	233.98	220.06
3705	232.84	235.71	225.20	231.53	220.23
3710	232.80	236.65	225.16	239.46	220.18
3715	232.68	236.51	225.04	239.33	220.11
3720	233.07	237.03	225.39	239.90	220.26
3725	233.47	237.50	225.73	240.41	220.48
3730	232.98	236.94	225.30	239.83	220.25
3735	231.76	235.35	224.34	238.07	219.81
3740	231.09	233.41	224.04	235.46	220.15
3745	232.28	233.03	225.50	233.94	221.65
3750	235.16	234.61	228.39	233.94	224.46
3755	238.32	237.07	231.61	235.16	227.60
3760	243.66	242.43	237.07	239.30	233.01
3765	247.80	246.41	240.81	242.72	236.65
3770	250.62	249.32	243.39	245.29	239.08
3775	253.84	252.61	246.17	248.23	241.59
3780	254.59	253.37	246.80	248.90	242.13
3785	255.53	254.33	247.57	249.74	242.77

TABLE V-1: Continued

WAVE NUMBER	1	MODEL 2	ATMOSPHERE		
			3	4	5
3790	255.15	253.95	247.27	243.42	242.52
3795	252.79	251.54	245.30	247.28	240.32
3800	249.78	242.44	242.71	244.53	238.47
3805	247.40	245.96	241.56	242.36	236.48
3810	245.26	243.74	239.50	241.45	234.58
3815	244.17	242.57	237.57	233.46	233.54
3820	243.23	241.51	236.68	233.63	232.66
3825	242.63	240.95	236.10	233.09	232.07
3830	242.32	240.64	235.81	237.84	231.70
3835	242.02	240.33	235.52	237.59	231.51
3840	242.34	240.66	235.82	237.85	231.81
3845	242.82	241.15	236.28	233.25	232.25
3850	243.13	241.47	236.58	233.52	232.56
3855	243.29	241.64	236.73	238.68	232.71
3860	243.61	241.93	237.04	238.96	233.02
3865	243.93	242.32	237.34	233.24	233.32
3870	244.42	242.83	237.80	239.67	233.78
3875	245.06	243.51	238.40	240.24	234.38
3880	246.03	244.53	239.31	241.13	235.20
3885	247.36	245.93	241.53	242.32	236.47
3890	250.11	248.81	243.00	244.83	238.75
3895	253.70	252.48	246.06	248.10	241.51
3900	255.93	254.74	247.90	251.10	243.06
3905	257.82	256.62	248.41	251.81	244.23
3910	258.58	257.33	250.01	252.51	244.76
3915	258.41	257.21	249.87	252.35	244.65
3920	257.84	256.65	249.43	251.84	244.31
3925	257.67	256.47	249.29	251.68	244.13
3930	257.86	256.67	249.45	251.86	244.31
3935	258.63	257.43	250.04	252.55	244.79
3940	259.97	258.77	251.08	253.77	245.53
3945	260.54	259.35	251.52	254.29	245.92
3950	263.03	261.81	253.39	256.56	247.26
3955	265.32	264.07	255.04	258.67	248.39
3960	267.41	266.12	256.50	260.62	249.33
3965	270.03	268.63	258.25	263.07	250.41
3970	272.42	270.99	259.75	265.29	251.29
3975	275.12	273.53	261.34	267.76	252.17
3980	278.42	276.52	263.13	271.64	253.13
3985	281.34	279.03	264.50	273.10	253.86
3990	282.42	280.02	265.11	273.98	254.11
3995	283.02	280.53	265.38	274.47	254.25
4000	282.88	280.41	265.32	274.36	254.22

TABLE V-1: Continued

```

13 PROGRAM LOWTRAN (TAPE2,TAPE4,TAPE5,TAPE6)
14 DIMENSION WTAU(34,8),TTAU(34)
15 COMMON P(5,34),T(5,34),WH(5,34),WO(5,34),HZ1(34),HZ2(5),Z(34)
16 COMMON C1(2587),C2(1575),C3(540),C4(133),C5(15),C8(102)
17 COMMON TR(67),FW(57),FO(67),HZ(2),EH(8,34),VH(8),W(8),TX(8)
18 COMMON /TRNCOM/ IATM,NL,I,IV
19 *****
20 C J.E.A.SELBY AFRL(CPI)
21 C PROGRAM LOWTRAN1 CALCULATES THE TRANSMITTANCE OF THE ATMOSPHERE
22 C FROM 350 CM-1 TO 4000 CM-1 (0.2 TO 25 MICRONS) AT 20 CM-1
23 C SPECTRAL RESOLUTION OF A LINEAR WAVENUMBER SCALE.
24 *****
25 400 FORMAT(3I3)
26 408 FORMAT(/28H HORIZONTAL PATH, ALTITUDE =,F7.2,11H KM,RANGE =,F7.2,
27 1 3H KM )
28 409 FORMAT(/50H SLANT PATH BETWEEN ALTITUDES H1 AND H2 WHERE H1 =,
29 1 F7.2,8H KM H2 =,F7.2,18H KM,ZENITH ANGLE =,F7.3,8H DEGREES )
30 410 FORMAT(/30H SLANT PATH TO SPACE FROM ALTITUDE H1 =, F7.2,18H KM,
31 1ZENITH ANGLE =,F7.3,8H DEGREES )
32 411 FORMAT(/18H MODEL ATMOSPHERE ,I1, 11H = TROPICAL)
33 412 FORMAT(/18H MODEL ATMOSPHERE ,I1, 21H = MIDLATTITUDE SUMMER)
34 413 FORMAT(/18H MODEL ATMOSPHERE ,I1, 21H = MIDLATTITUDE WINTER)
35 414 FORMAT(/18H MODEL ATMOSPHERE ,I1, 21H = SUB-ARCTIC SUMMER)
36 415 FORMAT(/18H MODEL ATMOSPHERE ,I1, 21H = SUB-ARCTIC WINTER)
37 416 FORMAT(/18H HAVE MODEL ,I1, 3H = ,A5,13H VISUAL RANGE )
38 417 FORMAT(/21H FREQUENCY RANGE V1=,F7.2,13H CM-1 TO V2 =,F7.1,14H
39 1CM-1 FOR DV =,F6.1,7H CM-1 ,//)
40 PLANCK(T,V) = 1.19105E-12*V**3/(EXP(1.43879*V/T) - 1.0)
41 HZ(1) = 5H23 KM
42 HZ(2) = 5H 5 KM
43 CALL READ5
44 *****
45 C *****

```


Reproduced from
best available copy.

550
555
560
565
570
575
580
585
590
595
600
605
610
615
620
625
630
635
640
645
650
655

```

V2 = 4000.0
OV = 5.0
IF(ITYPE.EQ.1) WRITE(5,403) H1,RANGE
IF(ITYPE.EQ.2) WRITE(5,409) H1,H2,ANGLE
IF(ITYPE.EQ.3) WRITE(5,410) H1,ANGLE
M=MODEL
IF(M.EQ.1) WRITE(5,411) M
IF(M.EQ.2) WRITE(5,412) M
IF(M.EQ.3) WRITE(5,413) M
IF(M.EQ.4) WRITE(5,414) M
IF(M.EQ.5) WRITE(5,415) M
WRITE(6,416) IHAZE,H7(IHAZE)
WRITE(6,417) J1,J2,OV
IF(IHAZE.F0.1) GO TO 4
DO 3 I=1,5
3 HZ1(I)=HZ2(I)
4 CONTINUE
C*** NOW DEFINE CONSTANT PRESSURE PATH QUANTITIES EH(1-8)
DO 9925 ITAU = 1, 31
H1 = Z(ITAU)
DO 5 J=1,NL
PS=P(M,I)/1J13.0
TS=273.0/T(M,I)
X= PS*T
PT=PS*SQRT(TS)
D=0.1*WH(M,I)
EH(1,I)=D*PT**0.9
EH(2,I)=X*PT**0.75
EH(3,I)=40(M,I)*PT**0.4
EH(4,I)=1.9*PT*X
PPW=4.56E-6*WH(M,I)*T(M,I)
EH(5,I)=(PPW+0.00E*(PT-PPW))*D

```

```

EH(6,I)=X
EH(7,I)=3.53355-4X474(I)
EH(8,I)=40(4,I)
5 CONTINUE
IK=1
X=H1
6 DO 7 I=1,NL
  J1=I
  IF(X-Z(I))3,1,2
7 CONTINUE
8 J2=J1
  IF(X.GT.Z(NULL)) Y = Z(NULL)
  J1=J1-1
  J11=J1
  FAC=(X-Z(J1))/(Z(J2)-Z(J1))
  IF(XK.EQ.1) J11=J2
  DO 9 K=1,4
    EH(K,J11)=EH(K,J1)*(C1(K,J2)/EH(K,J1))**FAC
9 CONTINUE
10 IF(ITYPE.EQ.1) GO TO 5
  IF(XK.EQ.1) GO TO 11
  J2=ILL
  IF(ITYPE.EQ.3) GO TO 12
  IJK=J1
  IK=1
  X=H2
  GO TO 6
11 J1=IJK
  J2=J2-1
12 CONTINUE
  DO 13 K=L,3
    VH(K)=J1
  13

```

070
 080
 090
 100
 110
 120
 130
 140
 150
 160
 170
 180
 190
 200
 210
 220
 230
 240
 250
 260
 270
 280
 290
 300
 310
 320
 330
 340
 350
 360
 370
 380
 390
 400
 410
 420
 430
 440
 450
 460
 470
 480
 490
 500
 510
 520
 530
 540
 550
 560
 570
 580
 590
 600
 610
 620
 630
 640
 650
 660
 670
 680
 690
 700
 710
 720
 730
 740
 750
 760
 770
 780
 790
 800
 810
 820
 830
 840
 850
 860
 870
 880
 890
 900
 910
 920
 930
 940
 950
 960
 970
 980
 990

Reproduced from
best available copy.

```

13 CONTINUE
IF (J2.LT.NLL) GO TO 15
NOW DEFINE GEOMETRICAL QUANTITIES J4(1-N)
DO 19 K=1,N
EV=(Z(NLL)-Z(NLL-1))*H(K,NLL)
IF (FH(K,NLL).EQ.F4(K,NLL-1)) GO TO 14
EV=EV/ALOG(EH(K,NLL-1)/EH(K,NLL))
14 VH(K)=EV*VH(K)
15 CONTINUE
I=NLL
IF (J2.EQ.NLL) J2=NLL-1
16 DO 19 I=J1,J2
X=Z(I)
IF (I.EQ.J1) X=41
OZ=Z(I+1)-X
IF (I.EQ.J2) OZ=42-X
DO 19 K=1,N
IF (E4(K,I).EQ.EH(K,I+1)) GO TO 17
EV=OZ*(E4(K,I)-E4(K,I+1))/ALOG(E4(K,I)/E4(K,I+1))
GO TO 18
17 EV=OZ*EH(K,I)
18 VH(K)=VH(K)+EV
19 CONTINUE
GO TO 22
DO 20 21 K=1,N
W(K)=RANGE*EH(K,J1)
21 CONTINUE
GO TO 24
IF (ANGLE.GT.90) GO TO 24
22 V=3.14159*ANGLE/180.0
DO 23 K=1,N
W(K)=W(K)/COS(V)

```

1290
1300
1310
1320
1330
1340
1350
1360
1370
1380
1390
1400
1410
1420
1430
1440
1450
1460
1470
1480
1490
1500
1510
1520
1530
1540
1550
1560
1570
1580
1590
1600

```

23 CONTINUE
C*** INSERT ENTH CORRECTION AND REFRACTION
24 CONTINUE
    DO 9925 JTAU = 1, 9
        WTAU(JTAU, JTAU) = W(JTAU)
9925 CONTINUE
    I=1
    IV1=V1/5.0
    IV2=V2/5.0+.30
    IV1=5*IV1
    IV2=5*IV2
    IF(IV1.LT.30) IV1=30
    IF(IV2.GT.5000) IV2=5000
    IF(IV.LT.5.0) IV=5.0
    IOV=IV
    IV=IV1-IV
    ICONT=1
C*** BEGINNING OF TRANSMITTANCE CALCULATIONS
30 IV=IV+IOV
    IF(ICOUNT.EQ.0) GO TO 31
    IF(ICOUNT.EQ.55) GO TO 31
    GO TO 32
31 ICONT=0
    WRITE (5,26)
32 CONTINUE
    V = IV
    SUMTAU = 0.0
    DO 9940 KTAU = 1, 9
        FACTAU = 1.0/COS(ACOS(SORT((2.0*KTAU - 1.0)/10.0)))
    DO 9940 JTAU = 1, 74
    DO 9933 JTAU = 1, 9
        W(JTAU) = FACTAU*WTAU(JTAU, JTAU)

```


9933	CONTINUE	1933
	CALL TRANS	1943
	TTAU(ITAU) = TX(2)	1950
	IF (ITAI .NE. 1) GO TO 9935	1959
	SUMTAU = SUMTAU + BLANK(T(M,1),V)*TTAU(1)	1973
	GO TO 9939	1982
9935	CONTINUE	1992
	TMTAU = (T(M,ITAU) + T(M,ITAU-1))*J.5	2003
	SUMTAU = SUMTAU + BLANK(TMTAU,V)*(TTAU(ITAU) - TTAU(ITAU-1))	2013
9938	CONTINUE	2022
9940	CONTINUE	2030
	SUMTAU = 2.2*SUMTAU	2040
	ICOUNT = ICOUNT + 1	2050
	V = IV	2060
	ALAM=1.0E+04/V	2070
	TMTAU = 1.43379*V/ALAM(1.13106E-12*V**3/SUMTAU + 1.0)	2080
	WRITE (5,430) IV,ALAM,TMTAU,SUMTAU	2090
	WRITE (2,430) IV,ALAM,TMTAU,SUMTAU	2100
430	FORMAT (1X,I6,F12.4,F8.2,1PE12.3)	2110
	IF (IV.GE.IV2) GO TO 75	2120
	GO TO 30	2130
75	CONTINUE	2140
	STOP	2150
	END	2160

```

SUBROUTINE TRANS
COMMON P(5,34),T(5,34),WM(5,34),M(5,34),M21(34),M22(5),7(34)
COMMON C1(2581),C2(1575),C3(541),C4(133),C5(15),C6(112)
COMMON T2(57),FW(57),FO(57),H2(2),E4(3,34),VH(5),W(3),TX(2)
COMMON V2(100),TATM,NL,M,IV
DO 33 K=1,9
TX(K)=J.0
IF(K.LT.+) TX(K)=1.0
33 CONTINUE
SUM=0.0
V=IV
I=(IV-15)/5+1
IF(IV.LT.1400) GO TO 41
IF(IV.LT.2740) GO TO 48
C***** MOLECULAR SCATTERING
C6=9.807E-25*(V**4.0117)
TX(6)=C6*W(6)
SUM=SUM+TX(6)
IF(IV.LT.9200) GO TO 53
IF(IV.LT.13000) GO TO 52
C***** UV 1700E
IF(IV.LE.23400) GO TO 34
IF(JV.GE.27500) GO TO 35
GO TO 70
34 XX=200.0
XI=(V-13100.0)/XX+1.0
L1=1
L2=53
GO TO 36
35 XX=500.0
XI=(V-27500.0)/XX+5.0
L1=57

```

```

L2=132
36 DO 37 N=L1,L2
   XD=XI-FLJAT(N)
   IF(XD)39,39,37
37 CONTINUE
38 TX(9)=W(3)*CA(N)
   GO TO 40
39 TX(8)=C3(N)+XD*(C3(N)-C8(N-1))
   TX(8)=W(3)*TX(8)
40 SUM=SUM+TX(8)
   A=C8(N)
   IF(IV.GT.1450) GO TO 70
   GO TO 51
C***** WATER VAPOR CONTINUUM
41 IF(IV.LE.870) GO TO 53
   IF(IV.LT.730) GO TO 45
42 XI=(V-700.)/50.+1.
   DO 43 NH=1,15
   XH=XI-FLJAT(NH)
   IF(XH)45,44,43
43 CONTINUE
44 TX(5)=C5(NH)
   GO TO 47
45 TX(5)=C5(NH)+XH*(C5(NH)-C5(NH-1))
   GO TO 47
46 TX(5)=(V-870.)*C.33
47 TX(5)=W(5)*TX(5)
   SUM=SUM+TX(5)
   A=C5(NH)
   GO TO 53
C***** NITROGEN CONTINUUM
48 IF(IV.LT.2380) GO TO 53

```

330
340
350
360
370
380
390
400
410
420
430
440
450
460
470
480
490
500
510
520
530
540
550
560
570
580
590
600
610
620
630
640

Reproduced from
best available copy.

```

K4=I-346
TX(4)=C4(K4)+V(4)
SUM=SUM+TX(4)
A=C4(K4)
GO TO 53
C***** WATER VAPOR
50 IF(IV.LT.12800.AND.IV.GE.12875) GO TO 51
   IF(IV.LE.14520.AND.IV.GE.13400) GO TO 52
   GO TO 57
51 I=I-135
52 GO TO 53
53 I=I-255
54 K1=1
   WS1=ALOG10(W(1))+C1(T)
   IF(WS1.LT.-2.3463) GO TO 57
   IF(WS1.GT.3.5582) GO TO 56
   IF(WS1.GT.2.0) K1=4
   DO 54 K=K1,67
   IF(WS1.LE.FW(K)) GO TO 55
54 CONTINUE
55 TX(1)= TR(K)+(TR(K-1)-TR(K))* (FW(K)-WS1)/(FW(K)-FW(K-1) )
   GO TO 57
56 TX(1)=0.0
57 CONTINUE
C***** UNIFORMLY MIXED GASES
   IF(IV.LT.12600.AND.IV.GE.5000) GO TO 58
   IF(IV.LT.13100.AND.IV.GT.12370) GO TO 58
   GO TO 6+
58 J=I-30
   GO TO 60
59 J=(IV-12350)/3+1514
60 CONTINUE

```



```
K1=1
WS2=ALOG10(W(2))+C2(.J)
IF(WS2.LT.-2.3468)GO TO 64
IF(WS2.GT.3.5582)GO TO 63
IF(WS2.GT.2.0) K1=40
DO 61 K=K1,67
IF(WS2.LE.FW(K)) GO TO 62
51 CONTINUE
52 TX(2)= TP(K)+(TP(K-1)-TP(K))*(FW(K)-WS2)/(FW(K)-FW(K-1))
GO TO 64
53 TX(2)=0.7
54 CONTINUE
C***** OZONE
IF(IV.LT.575.0P.TV.GT.3270) GO TO 63
L=I-45
K1=1
WS3=ALOG10(W(3))+C7(L)
IF(WS3.LT.-1.5778)GO TO 69
IF(WS3.GT.3.9345)GO TO 67
IF(WS3.GT.1.5) K1=76
DO 65 K=K1,67
IF(WS3.LE.FO(K)) GO TO 66
55 CONTINUE
56 TX(3)= TP(K)-(TP(K)-TP(K-1))*(FO(K)-WS3)/(FO(K)-FO(K-1))
GO TO 68
57 TX(3)=0.7
58 CONTINUE
C***** AEROSOL EXTINCTION
70 C7=3.75+E-5*(V**3.6543)
IF(IV.LT.3000)GO TO 71
GO TO 72
71 C7=C7+(6.8E-7)*(3.0E.7-V)
```

970
980
990
1000
1010
1020
1030
1040
1050
1060
1070
1080
1090
1100
1110
1120
1130
1140
1150
1160
1170
1180
1190
1200
1210
1220
1230
1240
1250
1260
1270
1280

```

72 TX(7)=C7*W(7)
   SUM=SUM+TX(7)
TX(8)=SUM
4*3 FORMAT( 3(I3,F10.2),5F13.3)
DO 75 K=4,9
  IF(TX(K).EQ.0.0) GO TO 74
  IF(TX(K).LE.0.1) GO TO 73
  TX(K)=EXP(-TX(K))
  GO TO 75
73 TX(K)=1.-TX(K)+0.5*TX(K)*TX(K)
  GO TO 75
74 TX(K)=1.0
75 CONTINUE
TX(9)=TX(1)*TX(2)*TX(3)*TX(4)
IF(14.5E-13GT TX(9)) TX(9)=TX(4)
  RETURN
  END

```

```

1390
1395
1400
1405
1410
1415
1420
1425
1430
1435
1440
1445
1450

```



```

100 SURROUTINE READ =
110 COMMON O(5,3+),T(5,3+),WH(5,3+),WO(5,3+),H71(3+),H72(5),7(3+)
120 COMMON Z1(2580),Z2(1575),C3(540),C4(133),C5(15),C9(112)
130 COMMON TP(57),FW(57),FO(57),HZ(2),EH(8,34),WH(8),W(8),TX(8)
140 COMMON /TPNCOM/ TATM,NL,4,IV
150 FORMAT(3I3)
160 FORMAT(7E10.3)
170 FORMAT(F6.1,2(E10.3,F6.1,2E10.1))
180 FORMAT(F6.1,E10.3,F6.1,2E10.1,E14.4)
190 FORMAT(+ (F6.3,2F7.4))
200 FORMAT(15F5.2)
210 FORMAT(3F9.2)
220 HZ(1) = 5423 K1
230 HZ(2) = 545 KM
240 READ (5,400) IATM,NL
250 IF(IATM.EF.5) GO TO 511
260 READ (5,401)(H72(T),T=1,5)
270 J=-1
280 DO 500 K0=1,2
290 K1=J+2
300 K2=K1+1
310 J=1
320 DO 500 I=1,NL
330 READ (5,402)Z(T),(P(K,I),T(K,I),WH(K,I),WO(K,I),K=K1,K2)
340 CONTINUE
350 K=IATM
360 DO 502 I=1,NL
370 READ (5,403)Z(I),O(K,I),T(K,I),WH(K,I),WO(K,I),H71(I)
380 READ (5,404)(TP(I),FW(I),FO(I),I=1,57)
390 READ (5,405)(C1(I),I=1,2580)
400 READ (5,405)(C2(I),I=1,1575)
410 READ (5,405)(C3(I),I=1,540)

```

330
340
350
360
370

READ (5,415) (C4(J), I=1,133)
READ (5,435) (C5(I), I=1,15)
READ (5,436) (C8(T), T=1,102)
RETURN
END

Program SPCTRA

Purpose:

SPCTRA computes the spectral radiances in the 5 to 25 μm interval corresponding to the band radiances computed by BCKGND. The input data to SPCTRA are the molecular band line constants, molecular vibrational level and band constants used by, and vibrational population and band radiance data generated by BCKGND. In its present form, SPCTRA computes spectral radiances between 2.5 and 25 μm for limb views and endo-atmospheric zenith angles of 0 and 90 degrees at 5 km intervals between 60 and 200 km.

Program Flow:

When program execution begins, values are assigned to the integer variables NOUT, NLN and NALT and the subroutine ROTATE, which reads in data for the molecular lines, is called. The outer DO range ending with statement 500 is entered. The DO parameters are fixed at present to produce two sets of spectra, using night and day input from program BCKGND. The program may be made more flexible by reading in DO parameters prior to execution of the DO statement. The variable BLAM is set to 5.0 and the outer DO range ending with statement 105 is entered. The effect of the first two statements is to set up a table of wavenumbers at 2 cm^{-1} intervals between 2.5 and 25 μm in real array AVLAM. These are the finest wavenumbers at which spectral radiances may be printed out. The inner DO range ending with statement 105 sets the values of output spectral radiances equal to zero.

The DO range ending with statement 110 sets temperature values in array TEMP to those corresponding to the U.S. Standard Atmosphere, 1962. Temperature values may also be read in prior to execution of the first DO statement. Following final execution of this DO range, temperatures are printed out.

Next, the number of molecular species is read in and stored in integer variable NSPTOT. The outer DO range ending with statement 400 is entered and executed NSPTOT times. Within this DO range, molecular vibrational level and band data and vibrational population data are read in and mean temperatures and total number of molecules per unit area in the vertical and horizontal directions are computed for each vibrational state. Total band radiances corresponding to limb viewing and vertical and horizontal endo-atmospheric viewing are read in. Relative line radiances are computed and normalized to the total band radiances. The spectra corresponding to the normalized line radiances are computed and stored in arrays SPECA, SPECB and SPECC. Details of these computations are given below.

The code number of the species ISP is read in. The number of vibrational levels NLEVEL, the number of bands NBAND and the molecular weight RM are read in. In the DO range ending with statement 210, the level description codes LSC and LCC, the energy and the mean rotational constant for each vibrational level are read in. In the DO range ending with statement 220 the band description codes LBC and LBU and the band strength

for each band are read in. The number of altitudes NALT for which vibrational populations are computed for the species and the number of altitudes NRLEV for which band radiances are computed by BCKGND are read in. Vibrational level populations are read in and stored in array CON.

The mean temperatures and total number of molecules per square centimeter in the vertical and horizontal directions at 5 km intervals between 60 and 200 km are determined in the DO range ending with statement 129. The product of temperature and vibrational level population is computed in the DO range ending with statement 112. The integrals of total number of molecules and the product of temperature and number density in the vertical direction are computed in the DO range ending with statement 120. Simpson's rule integration is used. The total number of molecules in a given vibrational level above a given altitude is stored in array COLCNT. The corresponding mean temperatures, obtained by dividing the integral of the product of temperature and number density by the integral of number density, are stored in array AVTEMP. After exit from DO range, the column counts and temperatures are printed out.

The DO range ending with statement 128 performs a similar computation for column counts and mean temperatures in the horizontal direction. The integrations required are performed in function QINT. Upon exit from this DO range, column counts stored in array HORCNT and mean temperatures stored in array BVTEMP are printed out.

The inner DO range ending with statement 400 is now entered and executed for each band. This DO range controls the computation of the spectra.

The altitude HT, the limb band radiance RADC, and endoatmospheric radiances RADA (upward direction) and RADB (horizontal direction) are read in the DO range ending with statement 230. Band information is computed from band and level constants. A test is made on the species code ISP to determine whether the molecule is linear or nonlinear.

Following the test of ISP, if the molecule is linear and is not in McClatchey's tabulation, line positions are computed in subroutine ROTPOS. The DO range ending with statement 250 is entered and executed for each of the 20 altitudes for which spectra are computed. Line radiances are computed in subroutine ROTSTR for vertical endo-atmospheric viewing. Successive calls to subroutine FILTER compute the spectral contributions from lines in the P, Q and R branches. The sequence of calls to ROTSTR and FILTER is repeated for endo-atmospheric viewing in the horizontal direction and for limb viewing. Upon exit from this DO range, control is transferred to statement 280.

If the test on ISP determines that the molecular line data is available control is transferred to statement 260 and the DO range ending with statement 270 is executed for each of the 28 altitudes for which spectra are computed. Spectra are generated from the line radiances by calls to subroutine WATSTR and FILTER, for each of the three

viewing conditions.

Following the final execution of the DO ranges ending with statement 400, the spectra are printed out in the order endo-atmospheric viewing in the upward direction, endo-atmospheric viewing in the horizontal direction and limb viewing.

Upon final execution of the DO range ending with statement 500, the program halts with a STOP statement.

Mnemonic Variables:

AVLAM	Real array in which output wavenumbers are stored.
AVTEMP	Real array in which mean temperatures in the vertical direction are stored.
BV	Real array in which rotational constants for each vibrational level are stored.
BVTEMP	Real array in which mean temperatures in the horizontal direction are stored.
COLCNT	Real array in which total number of molecules per square centimeter above 60, 65, ... 200 km in each vibrational level are stored.
CON	Real array in which number densities for each vibrational level are stored.
HHOLAM	Real array in which wavenumbers of band lines are stored.
HHOLSE	Real array in which lower state energies of band lines are stored.
HHOSTR	Real array in which strengths of lines are stored.
HORCNT	Real array in which total number of molecules per square centimeter in each vibrational level in the horizontal direction at altitudes 60, 65, ... 200 km are stored.

HRAD	Real array in which line radiances are stored.
P	Real array in which wavelengths of P branch of linear molecule are returned by subroutine ROTPOS.
PRAD	Real array in which products of number density and temperature are stored.
PS	Real array in which P branch line radiances are returned by subroutine ROTSTR.
Q	Real array in which Q branch line wavelengths are returned by subroutine ROTPOS.
QS	Real array in which Q branch line radiances are returned by subroutine ROTSTR.
R	Real array in which R branch line wavelengths are returned by subroutine ROTPOS.
RADA	Real array into which vertical direction and endo-atmospheric band radiances are read.
RADB	Real array into which horizontal direction endo-atmospheric band radiances are read.
RADC	Real array in which limb view band radiances are read.
RCM	Real array into which vibrational level energies are read.
ROTEA	Real array used by subroutines ROTATE and WATSTR, stores factors needed to compute line radiances in water vapor pure rotational spectrum.
ROTLAM	Real array in which water vapor pure rotational line wavelengths are stored.
ROTLSE	Real array in which lower state energies of water vapor pure rotational lines are stored.
ROTST	Real array in which absorption strengths of water vapor pure rotational lines are stored.
RS	Real array in which R branch line radiances are returned by subroutine ROTSTR.

SPECA	Real array in which spectral radiances for vertical viewing endo-atmospheric geometry are generated.
SPECB	Real array in which spectral radiances for endo-atmospheric horizontal viewing are generated.
SPECC	Real array in which spectral radiances for limb viewing are generated.
STR	Real array used to store band strengths.
TEMP	Real array used to store atmospheric temperatures.
BLAM	Real variable used as temporary storage during generation of values in array AVLAM.
CENTER	Real variable used to store wavenumber of band center.
HT	Real variable into which altitudes at which band radiances are computed by BCKGND are read.
H1, H2, H3, H4, H5	Real variables used to store distance increments used in computing total column counts and mean temperatures in the horizontal direction.
RBASE	Real variable used to store distance of base altitude from center of earth in computing horizontal column counts.
RB2	Real variable used to store value of $RBASE^{**2}$.
RM	Real variable used to store value of molecular weight.
RTOP	Real variable used to store distance from center of earth of given altitude level.
SNB	Real variable used to store current value of band strength.
STH	Real variable used as temporary storage is computing horizontal column counts.
SVH	Real variable used as temporary storage in computing horizontal column counts.
TC	Real variable used to accumulate integral of number density in computing vertical column counts.

TCH	Real variable used to accumulate integral of number density in computing horizontal column counts.
TP	Real variable used to accumulate integral of product of temperature in the vertical direction.
TPH	Real variable used to accumulate integral of product of temperature and number density in computing mean temperature in the horizontal direction.
LBC	Integer array storing level numbers of initial and final states of a band.
LBU	Integer array storing band type and symmetry information.
LCC	Integer array storing vibrational level information.
LSC	Integer array storing vibrational level information.
I	Integer variable used as index in DO loops.
ISP	Integer variable into which species identification code is read (2 for CO ₂ , 3 for H ₂ O, 4 for NO, 5 for N ₂ O and 6 or 7 for ozone).
J	Integer variable used as index in DO loops.
K	Integer variable (set equal to 28 in current program) used as final parameter in DO statement controlling computation of column counts and mean temperatures. The value of K is the number of altitudes for which spectra are computed.
KB	Integer variable used to store band type code.
KK	Integer variable used as final parameter in DO range ending with statement 125, computed from K and I.
KL	Integer variable used to store band symmetry code.
NA	Integer variable used as altitude level index in computing horizontal column counts.
NALT	Integer variable storing total number of altitude levels.

NB	Integer variable used as index for number of current band.
NBAND	Integer variable storing total number of bands considered for a given species.
NBC	Integer variable used to store current value of LBC.
NCASES	Integer variable used as index for spectrum set.
NF	Integer variable used as index for lower vibrational state of band.
NI	Integer variable used as index for upper vibrational state of band.
NL	Integer variable used as index for vibrational level number.
NLEVEL	Integer variable in which is stored total number of vibrational levels for a molecular species.
NLN	Integer variable controlling number of lines treated in each branch of a band of a linear molecule, set to 100 in current program.
NRLEV	Integer variable into which is read number of altitudes at which band radiances for a given species are computed by BCKGND.
NSP	Integer variable used as index for DO range executed NSPTOT times.
NSPTOT	Integer variable into which is read total number of species to be included in a spectrum.
NZ	Integer variable used as altitude index in DO loops.


```

C      COMPUTE MEAN TEMPERATURES AND COLUMN COUNTS
      K = NRLEV
      DO 129 J = 1, NLEVEL
      DO 112 I = 1, NALT
      PFOD(I) = CON(I,NL)*TEMP(I)
112 CONTINUE
      TP = 1.0
      TC = 1.0
      NA = NALT
      DO 120 I = 1, K
      TP = TP + SIMP(PROD(NA - 2),1.0E+5,2)
      TC = TC + SIMP(PROD(NA - 3),1.0E+5,3) + SIMP(PROD(NA - 5),1.0E+5,3)
      NA = NA - 5
120 CONTINUE
      RBASE = 6.431E+8
      DO 128 I = 1, K
      TP4 = 0.0
      TC4 = 0.0
      NA = NALT
      RB2 = RBASE*RBASE
      RTOP = 6.431E+8 + NALT*1.0E+5
      SV4 = SQRT(RTOP*RTOP - RB2)
      KK = K - I + 1
      DO 125 J = 1, KK
      RTP = RTOP - 1.0E+5
      STH = SQRT(RTOP*RTOP - RB2)
      H5 = SVH - STH

```

```

SV4 = STH
RTOP = RTOP - 1.0E+5
ST4 = SQRT(RTOP*RTOP - RB2)
H4 = SV4 - STH
SV4 = STH
RTOP = RTOP - 1.0E+5
ST4 = SQRT(RTOP*RTOP - RB2)
H3 = SV4 - STH
SV4 = STH
RTOP = RTOP - 1.0E+5
ST4 = SQRT(RTOP*RTOP - RB2)
H2 = SV4 - STH
SV4 = STH
RTOP = RTOP - 1.0E+5
ST4 = SQRT(ABS(RTOP*RTOP - RB2))
H1 = SV4 - STH
SV4 = STH
TP4 = TPH + QINT(PROD(NA - 2), H4, H5, 2)
1 + QINT(PROD(NA - 3), H3, H4, 3) + QINT(PROD(NA - 5), H1, H2, 3)
TC4 = TCH + QINT(CON(NA - 2, NL), H4, H5, 2)
1 + QINT(CON(NA - 3, NL), H3, H4, 3) + QINT(CON(NA - 5, NL), H1, H2, 3)
NA = NA - 5
125 CONTINUE
HORCNT(I, NL) = TCH
BVIFMP(I, NL) = TPH/TCH
RBASE = RBASE + 5.0E+5
128 CONTINUE
129 CONTINUE
C ***** SET J VALUE
J = 1
C ***** OR SET UP DO LOOP
IF (ISP.NE. 3) GO TO 225
650
660
670
680
690
700
710
720
730
740
750
760
770
780
790
800
810
820
830
840
850
860
870
880
890
900
910
920
930
940
950
960

```


250	CALL FILTER (SPEC, QS, Q, NLN)	1290
	CALL FILTER (SPEC, RS, R, NLN)	1300
	CONTINUE	1310
	GO TO 400	1320
260	CONTINUE	1330
	IF (NR .GT. 10 .AND. ISP .EQ. 3) GO TO 400	1340
	CALL ROTATE (5, LINES)	1350
	CALL MATSTR (RADG(J), RM, 9, VTEMP(J, NF), 2.0*HOPCNT(J, NF), 2, LINES)	1360
	CALL FILTER (SPEC, HRAD, WVNUM, LINES)	1370
400	CONTINUE	1380
	WRITE (2, 16)	1390
	WRITE (2, 8) SPEC	1400
	WRITE (4, 8) SPEC	1410
500	CONTINUE	1420
	STOP	1430
6	FORMAT (6I6)	1440
8	FORMAT (1P6E11.3)	1450
14	FORMAT (1X)	1460
12	FORMAT (1P6E12.4)	1470
15	FORMAT (141)	1480
41	FORMAT (2I6, 5E12.4)	1490
42	FORMAT (8E10.4)	1500
43	FORMAT (F6.1, 3E17.4)	1510
	END	1520

Subroutine FILTER

Purpose: FILTER computes the contribution to spectral radiance from each line in a band or sub-band, in the interval $2.5\mu\text{m}$ to $25\mu\text{m}$. Provision is made for varying resolution in either wavelength or wavenumber space. Sufficient storage is provided to compute radiances at 2 wavenumber intervals with triangular slit resolution of 5 wavenumbers.

Method: FILTER searches an array of emission line strengths and assigns a weighted strength to an output wavenumber or wavelength.

Program Flow: The outer DO range ending with statement 150 controls the distribution of spectral radiance from the Ith of N given lines, and computes the indexes JS and JF of the first and last output points in array SPEC to which a given line contributes. The inner DO range ending with statement 120 computes the contribution of a given line to spectral radiance at output wavelengths or wavenumbers.

Inputs: RAD, WVLTH, N, KOMPUT

Output: SPEC

Mnemonic Variables:

SPEC	Real array into which spectra radiances are added at regular intervals between 2.5 and $25\mu\text{m}$ or 400 and 4000 wavenumbers.
------	---

RAD	Real array containing radiances of individual lines.
WULTH	Real array containing wavelengths of individual lines.
N	Integer variable containing number of lines in band or sub-band for which spectral radiance is to be computed.
KOMPUT	Integer variable which determines number of output spectral points and whether wavelength or wavenumber output is made.
RADT	Real variable used as temporary storage for radiance value of a single line.
RLAM	Real variable used temporary storage for wavelength value at which spectral radiance is computed.
RT	Real variable used as temporary storage for wavelength of a single line.
I	Integer variable used as index for outer DO loop which treats each line in turn.
J	Integer variable used as index for inner DO loop which assigns spectral contribution of each line to output wavelength.
JF	Integer variable used as final parameter in inner DO loop, index of greatest output wavelength for a given line.
JS	Integer variable used as initial parameter in inner DO loop, index of shortest output wavelength for a given line.

```

C
SUBROUTINE FILTER (SPEC,RAD,WVNUM,N)
FIVE WAVELENGTH RESOLUTION, TWO WAVELENGTH INTERVAL
DIMENSION SPEC(1801),RAD(450),WVNUM(450)
COMMON /ISPCOM/ ISP
DO 150 I = 1, N
  RT = WVNUM(I)
  IF (ISP .EQ. 4) RT = 1.0E+4/RT
  RADT = RAD(I)
  JS = (RT - 405.0)*0.5 + 2.0
  JF = (RT - 395.0)*0.5 + 1.0
  IF (JS .LT. 1) JS = 1
  IF (JF .GT. 1801) JF = 1801
  IF (JS .GT. JF) GO TO 150
  DO 120 J = JS,JF
    RNUM = (J - 1)*2.0 + 400.0
    SPEC(I) = SPEC(J) + (5.0 - ABS(RNUM - RT))*RADT*0.04
  120 CONTINUE
  150 CONTINUE
  RETURN
END

```

Subroutine ROTATE

Purpose:

Subroutine ROTATE is used to read in spectral line data from the compilation of McClatchey, et al. The input data consists of line positions and strengths for vibrational - rotational bands of water, carbon dioxide, ozone and nitrous oxide, and for the pure rotational spectrum of water. This data is processed for use by other subroutines.

Program Flow:

The DO range ending with statement 110 reads in data on the strongest lines in a vibration - rotation band. This data consists of the wave number of the line, the line strength at 296 K and the wavenumber of the lower rotational state. ROTATE converts the wavenumber to wavelength in μm stored in array HHOLAM, converts the line strength to units $\text{cm}^{-1}/\text{atm} - \text{cm}$ at 273.15k stored in array HHOSTR and stores the wavenumber of the lower state in array HHOLSE.

The rotational partition function for water vapor is computed next if water vapor data is being read. The DO range ending at statement 130 is used only for water vapor pure rotational lines and computes the wavelength (stored in array ROTLAM), Einstein A coefficient (stored in array EA), relative line strength in absorption at 273.15k (stored in array ROTST), relative line strength in emission at 273.15k (stored in array ROTEA) and the wavenumber of the lower rotational state (stored in array ROTLSE).

Mnemonic Variables:

EA	Real variable used to store Einstein A coefficient for water vapor pure rotational spectrum line.
EALC	Real variable used to store intermediate results in computing pure rotational line strengths in emission.
EALR	Real variable used to store intermediate results in computing pure rotational line strengths in absorption.
ENERGY	Real variable into which is read wavenumbers of pure rotational lines.
ENL	Real variable into which is read wavenumbers of lower states of pure rotational lines.
ENV	Real variable into which is read wavenumber of upper state of pure rotational line.
HHOLAM	Real array in which wavelengths of vibration - rotation band lines are stored.
HHOLSE	Real array in which wavenumbers of lower states of a vibration - rotation band are stored.
HHOSTR	Real array in which line strengths of vibration - rotation band are stored ($\text{cm}^{-2} - \mu\text{Tm}^{-1}$ STP).
ROTEA	Real array in which pure rotational line strengths in emission (273.15k) are stored.
ROTLAM	Real array in which pure rotational line wavelengths are stored.
ROTLSE	Real array in which lower state wavenumber of pure rotational lines are stored.
ROTST	Real array in which pure rotational line strengths in absorption are stored.

WVLTH	Real array in which wavelengths of vibration - rotation band lines are stored (redundant).
EAFAC	Real variable used to store pre-factor in computing Einstein A coefficients for pure rotational lines.
QR	Real variable in which is stored approximate rotational partition function for water vapor molecule.
QRFAC	Real variable into which is read prefactor for computing rotational partition function.
RA	Real variable into which is stored first water vapor rotational constant.
RB	Real variable into which is stored second water vapor rotational constant.
RC	Real variable into which is stored third water vapor rotational constant.
TEFAC	Real variable in which is stored exponential factor used in converting line intensities at 296K to line strengths at 273.15K.
TQFAC	Real variable in which is stored factor relating rotational function at 296K to that at 273.15K.
I	Integer variable used as index in DO loop.
NLINES	Integer variable into which is read number of lines included in pure rotational spectrum and in any single vibration - rotation band.

```

SUBROUTINE ROTATE (NIN,LINES)
COMMON /ISPCOM/ ISP
COMMON WNUM(2500),ENLS(2500),STR(2500),IRAD(2500)
READ (NIN,2) LINES
DO 120 I = 1, LINES
  READ (NIN,4) WNUM(I),STR(I),ENLS(I)
  STR(I) = 2.4793E+19*STR(I)
120 CONTINUE
  RETURN
2  FORMAT (1X,I8)
4  FORMAT (F10.3,1PE10.3,5X,0PF10.3)
END

```

```

10
20
30
40
50
60
70
80
90
100
110
120

```

Subroutine WATSTR

Purpose:

WATSTR computes the radiances of individual lines in vibration - rotation bands and in the pure rotational spectrum of water vapor. The radiances are computed with the assumption that the atmosphere in the line of sight may be treated as having uniform temperature. The radiances computed for the vibration - rotation bands are scaled to match the total band radiances produced by the BACKGROUND program. Absolute radiance values are computed for the water vapor pure rotational spectrum.

Program Flow:

Upon entry to WATSTR, a conversion factor TQFAC is computed for later use in computing the effect of charging rotational partition function with temperature. Control is then transferred to the appropriate part of the subroutine as determined by the value of N.

For computation of the radiances of lines in the water vapor pure rotational spectrum ($N = 1$), control is transferred to statement 100. A radiance factor RADFAC and an optical thickness factor TAUFAC are computed. Then the optical thickness and radiance values corrected for optical thickness and induced emission are computed for each line in the DO range ending with statement 110. Control is returned to the main program. Line constants generated by subroutine ROTATE are available in the

arrays of common area ROTCOM. Radiance values are returned in array HRAD.

Control is transferred to statement 200 for computation of radiances of lines in the other bands. An optical thickness factor TAUFAC and factor TEFAC used in computing populations of rotational states at temperature T are computed. The variable SUM, used to accumulate the sum of relative radiances, is set to zero. In the DO range ending with statement 210, the optical thickness of each line is computed and the relative radiance value, corrected for optical thickness, is computed and stored in array HRAD. The sum relative radiances is accumulated in SUM. Upon exit from this DO range, the total radiance RAD is divided by SUM and stored in RADFAC. In the DO range ending with statement 220, absolute radiance values are obtained and stored in array HRAD. Control is then returned to the main program.

Mnemonic Variables:

RAD	Real variable containing total band strength for vibration - rotation band.
RM	Real variable containing molecular weight of molecule.
T	Real variable containing value of temperature.
DEN	Real variable containing total number of ground state molecules per square centimeter in line of sight.
N	Integer variable determining whether entry to WATSTR results in computation for water vapor pure rotational spectrum (N = 1) or other band (N = 2).

HHOLAM	Real array, values as in ROTATE.
HHOLSE	Real array, values as in ROTATE.
HHOSTR	Real array, values as in ROTATE.
HRAD	Real array used to return radiance values of individual lines.
ROTEA	Real array, values as in ROTATE.
ROTLAM	Real array, values as in ROTATE.
ROTLSE	Real array, values as in ROTATE.
ROTST	Real array, values as in ROTATE.
HSTR	Real variable used as temporary storage in computing optical thickness.
RADFAC	Real variable in which is stored prefactor used in computing radiance values.
SUM	Real variable in which partial sums of relative radiances are accumulated.
TAU	Real variable in which optical thickness at line center is generated.
TAUFAC	Real variable in which prefactor for optical thickness is stored.
TEFAC	Real variable in which factor used in computing rotational populations is stored.
TQFAC	Real variable in which factor converting rotational partition function is stored.


```

10  SURROJINE WAISTR (RAD,RM,T,DEN,N,LINES)
20  COMMON /ISPCOM/ ISP
30  COMMON WNUM(2500),ENLS(2500),STR(2500),HRAD(2500)
40  TQFAC = (296.0/T)**1.5
50  IF (ISP.EQ.2) TQFAC = 296.0/T
60  GO TO (100,200,300), N
70
80  CONTINUE
90  RADFAC = 1.58065E-20*DEN*TQFAC
100 TAJFAC = 4.8815E-18*SQRT(RM/T)*TQFAC*DEN
110 DO 110 I = 1, LINES
120   HHOLAM = 1.0E+4/WNUM(I)
130   TAJ = TAJFAC*STR(I)*EXP(-1.43879*ENLS(I)/T)
140   * (1.0 - EXP(-14387.9/(HHOLAM*T)))
150   ROTEA = 2.8*STR(I)/HHOLAM**2
160   HRAD(I) = RADFAC*ROTEA*SFUN(TAU)
170   *EXP(-1.43879*(1.0E+4/HHOLAM + ENLS(I))/T)
180
190 CONTINUE
200 RETURN
210 CONTINUE
220 TAJFAC = 4.8815E-18*SQRT(RM/T)*DEN
230 TEFAC = (T - 296.0)/(T*296.0)*1.43879
240 SUM = 0.0
250 DO 210 I = 1, LINES
260   HSTR = TQFAC*STR(I)*EXP(TEFAC*ENLS(I))
270   HHOLAM = 1.0E+4/WNUM(I)
280   TAJ = TAJFAC*HHOLAM*HSTR
290   HPAD(I) = TAU*SFUN(TAU)*EXP(-14387.9/(HHOLAM*T))
300   * /HHOLAM**4
310   SUM = SUM + HRAD(I)
320 CONTINUE
    RADFAC = RAD/SUM
    DO 220 I = 1, LINES

```

330
340
350
360
370
380

HRAD(I) = HRAD(I)*RADFAC
220 CONTINUE
RETURN
300 CONTINUE
RETURN
END

Subroutine ROTSTR

Purpose: Subroutine ROTSTR computes the relative radiances of lines in the vibration - rotation bands of those linear molecules, which are not included in the line parameter compilation of McClatchey, et al. The radiances are corrected for effects of optical thickness, and absolute values then determined by normalizing to total band radiances computed by the BACKGROUND program. As for nonlinear molecules, a single temperature is assumed for the molecules in the line of sight.

Program Flow: Upon entry to ROTSTR, the reduced rotational temperature SIG is computed, relative strengths of the P, Q and R lines for $J = 0$ are assigned and values assigned to the increment of J values DJ and the variable J value AJ. Depending on the value of ND, relative strengths of rotational lines are computed in either the DO range ending with statement 110 (parallel transition) or the DO range ending with statement 120 (perpendicular transition). Control is transferred to statement 300 and the prefactor TAUFAC used in computing optical thickness is evaluated. The variable SUM which accumulates the sum of relative radiances is set to zero. In the DO range ending with statement 310, optical thicknesses for lines in the P, Q and R branches and relative radiances for these lines, corrected for the effects

of optical thickness, are computed. In the DO range ending with statement 320, absolute line radiances normalized to the total band radiance RAD are computed. Control is then returned to the main program.

Mnemonic Variables:

RAD	Real variable containing total band strength.
RM	Real variable containing molecular weight of molecule.
BVPP	Real variable containing mean rotational constant of lower vibrational state.
AJ	Real variable containing varying value of rotational quantum number J of lower vibrational state.
DJ	Real variable containing value of increment of rotational quantum number.
T	Real variable containing mean temperature of emitting layer.
DEN	Real variable containing number of molecules in lower state per square centimeter in line of sight.
STR	Real variable containing band strength at 300K.
PS	Real array in which radiances of lines in P branch are returned.
QS	Real array in which radiances of lines in Q branch are returned.
RS	Real array in which radiances of lines in R branch are returned.
NP	Integer variable determining whether band is parallel (NP = 1) or perpendicular (NP = 2).

ND	Integer variable determining whether all lines are present (ND = 1) or alternate lines are missing (ND = 2).
P	Real array containing wavelengths of lines in P branch.
Q	Real array containing wavelengths of lines in Q branch.
R	Real array containing wavelengths of lines in R branch.
FAC	Real variable used to store exponential factor in computation of line strengths.
PTAU	Real variable storing optical thickness in a P branch line.
QTAU	Real variable storing optical thickness in a Q branch line.
RADFAC	Real variable storing ratio of total band radiance RAD and sum of relative line radiances.
RTAU	Real variable storing optical thickness of R branch line.
SIG	Real variable storing reduced rotational temperature.
SUM	Real variable which accumulates sum of relative line radiances.
TAUFAC	Real variable storing prefactor used in computing optical thickness at line centers.


```

300 CONTINUE
TAFAC = 4.8815E-18*SQRT(RM/T)*DEN*STR/SUM
SUM = 1.0
DO 310 I = 1, 100
PTAU = PS(I)*P(I)*TAUFAC
QTAU = QS(I)*Q(I)*TAUFAC
RTAU = RS(I)*R(I)*TAUFAC
PS(I) = PTAU*SFUN(PTAU)*EXP(-14387.9/(P(I)*T))/P(I)**4
QS(I) = QTAU*SFUN(QTAU)*EXP(-14387.9/(Q(I)*T))/Q(I)**4
RS(I) = RTAU*SFUN(RTAU)*EXP(-14387.9/(R(I)*T))/R(I)**4
SUM = SUM + PS(I) + QS(I) + RS(I)
310 CONTINUE
RADFAC = RAD/SUM
DO 320 I = 1, 100
PS(I) = PS(I)*RADFAC
QS(I) = QS(I)*RADFAC
RS(I) = RS(I)*RADFAC
320 CONTINUE
RETURN
END

```

Subroutine ROTPOS

- Purpose: ROTPOS computes the wavelength of lines in the P, Q and R branches of the infrared vibrational - rotational bands of linear molecules neglecting spin and Λ or ℓ doubling. It is used for bands not included in the compilation of McClatchey, et al.
- Method: The line positions are computed using equations (IV, 19), (IV, 20) and (IV, 22) of Herzberg (1945). It should be noted that use of these simple formulae results in an error in line positions which may approach $0.1 \mu\text{m}$ for large J values in transitions between doublet states.
- Program Flow: Upon entry to ROTPOS, the auxiliary values BDIF, BSUM, RCENT and TRI used in the computation are computed from the band center position and the rotational constants. The initial J value is set to zero and provisions made for omitting alternate lines by setting DJ equal to ND. This latter starting condition means that the alternate lines omitted are always those with odd J values. The wavelengths of 100 lines in each branch in units μm are then computed in the DO range ending with statement 110. The wavelengths are printed out and control returned to the main program.

Mnemonic Variables:

AJ	Real variable in which current rotational quantum number J is stored.
BDIF	Real variable storing difference of rotational constants BVP and BVPP.
BSUM	Real variable storing sum of rotational constants.
DJ	Real variable storing increment of rotational quantum number.
RCENT	Real variable containing constant used in computing R branch line positions.
TRI	Real variable containing constant used in computing R branch line positions.
CENTER	Real variable giving the wave number of the band center.
BVP	Real variable giving the mean rotational constant of the upper vibrational state.
BVPP	Real variable giving the mean rotational constant of the lower vibrational state.
P	Real array in which wavelengths of the P branch are returned.
Q	Real array in which wavelengths of the Q branch are returned.
R	Real array in which wavelengths of the R branch are returned.
ND	Integer variable determining whether all lines in a band are present (ND = 1) or whether alternate lines are missing (ND = 2).

```

C
C
C
C
C
C
C
SUBROUTINE ROTPOS (CENTER,BVP,BVPP,P,Q,R,ND)
RTPOS COMPUTES ROTATIONAL LINE POSITIONS
CENTER IS BAND CENTER, CM*(-1)
BVP IS ROTATIONAL CONSTANT OF UPPER STATE
BVPP IS ROTATIONAL CONSTANT OF LOWER STATE
P,Q,P ARE ARRAYS RETURNING LINE POSITIONS
ND EQ. 1 FOR ALL LINES
ND EQ. 2 FOR ALTERNATE LINES
DIMENSION P(100),Q(100),R(100)
B0IF = BVP - BVPP
BSUM = BVP + BVPP
RCENT = CENTER + BVP + BVP
TPI = 3.0*BVP - BVPP
AJ = .0
DJ = 10
DO 110 I = 1, 100
P(I) = 1.0E+4/((B0IF*AJ - BSUM)*AJ + CENTER)
Q(I) = 1.0E+4/((B0IF*AJ + BSUM)*AJ + CENTER)
R(I) = 1.0E+4/((B0IF*AJ + TRI)*AJ + RCENT)
AJ = AJ + DJ
110 CONTINUE
RETURN
8 FORMAT (10F10.3)
15 FORMAT (1X)
END

```

FUNCTION SIMP (A,H,K)	10
DIMENSION A(3)	20
IF (K - 2) 100,110,120	30
CONTINUE	40
SIMP = (8.0*A(2) + 5.0*A(1) - A(3))*H/12.0	50
RETURN	60
CONTINUE	70
SIMP = (8.0*A(2) + 5.0*A(3) - A(1))*H/12.0	80
RETURN	90
CONTINUE	100
SIMP = (4.0*A(2) + A(1) + A(3))*H/3.0	110
RETURN	120
END	130

```

10      FUNCTION SFUN (TAU)
20      Y = ABS(TAU)
30      IF (T.GT. 4.0) GO TO 110
40      X = (T - 2.0)*0.5
50      SFUN = (((0.001061*X - 0.004288)*X + 0.013586)*X - 0.042491)
60      1 *X + 0.114932)*X - 0.267057)*X + 0.556495
70      RETURN
80      110 CONTINUE
90      IF (T.GT. 10.0) GO TO 120
100     X = (T - 7.0)/3.0
110     SFUN = (((0.000347*X - 0.001167)*X + 0.003149)*X - 0.009545)
120     1 *X + 0.028248)*X - 0.081972)*X + 0.247900
130     RETURN
140     120 CONTINUE
150     Y = ALOG(T)
160     X = 1.0/Y
170     SFUN = (((0.067876*X - 0.268698)*X + 0.264553)*X
180     1 - 0.253167)*X + 0.325368)*X + 1.128379)*SQRT(Y)/T
190     RETURN
200     END

```

```

10  FUNCTION QINT (A,H1,H2,K)
20  DIMENSION A(3)
30  HS = H1 + H2
40  IF (K - 2) 100,110,120
50  CONTINUE
60  QINT = ((A(2)*HS - A(1)*H2 - A(3)*H1)*H1/(5.)*H2*HS)
70  + (A(1) + A(2))*0.5)*H1
80  RETURN
90  CONTINUE
100 QINT = ((A(2)*HS - A(1)*H2 - A(3)*H1)*H2/(5.)*H1*HS)
110 + (A(2) + A(3))*0.5)*H2
120 RETURN
130 CONTINUE
140 QINT = (A(2)*HS - A(1)*H2 - A(3)*H1)*(H1**3 + H2**3)
150 /((6.)*HS*H1*H2) + (A(1)*H1 + A(2)*HS + A(3)*H2)*0.5
160 RETURN
170 END

```


PLOTTING PROGRAM

The plotting program, TRYCRT, which was developed under the previous contract, has been revised and adapted to use the pen and paper plotter in addition to the microform plotter. The version presented here is designed to read the output file produced by the spectral radiance program, SPCTRA. It consists of the main program, TRYCRT, and six subroutines, LINSICA, LOGSCA, LINAXS, LOGAXS, GRID and NULINE. In addition, it uses the AFCRL/CDC 6600 system subroutines which are needed to produce plots.

Array IDENT contains information required by the computer installation to identify the plotted graphs. The CDC 6600 subroutines are initialized by calls to subroutines PLTID3 and PLOT. The number of graphs to be plotted, NCASES, number of characters, NXL, in x-axis caption, x-axis caption, XBCD, number of characters, NYL, in y-axis caption, and y-axis caption, YBCD, are read in from cards and printed on the line printer. The DO loop ending with statement 400 is then executed for each graph to be produced. Minimum wavelength, WVMIN, and maximum wavelength, WVMAX, are read. Plotting constants INF, NX and NY are computed. Wavelengths are read from the SPCTRA output tape (channel 2) and stored in array AVLAM. An appropriate subset is then stored in array X. These are then scaled by subroutine LINSICA. Radiance data are then read from channel 2 and stored in array SPCTRA. An appropriate subset is selected and stored in array Y. Values in Y are scaled for plotting by a call to subroutine LOGSCA. Axes are drawn on all four sides of the graph by calls to subroutines LINAXS and LOGAXS. Calls to subroutine GRID place vertical and horizontal grid lines on the graph. Radiance values are further scaled in the DO loop ending

with statement 150. Radiance values are placed on the graph by calls to subroutine NULINE in the loop ending with statement 200. After each set of curves on a graph is produced, a call to subroutine PLOT prepares for a new graph. The DO loop ending with statement 250 is repeated three times, the first and second cycles plotting vertical and horizontal endoatmospheric radiances while the third plots limb viewing radiances. When only limb viewing radiances are desired, statement 250 should be placed immediately after the statement "READ (2) SPCTRA" on line TCRT 540.

Subroutines LINSKA and LOGSKA were written to provide automatic scaling of data points in a manner which would utilize maximum space on the graph. In addition to scaling data points, these subroutines generate values KONX, DX, MINY and MAXY which provide data which is used in the axis drawing subroutines LINAXS and LOGAXS and the grid drawing subroutine GRID. The subroutine NULINE was written to replace the standard AFCRL/CDC 6600 subroutine LINE which draws straight lines between plots. NULINE permits points to be plotted a limited distance outside the graph boundaries if the data for a graph covers more than 9 orders of magnitude.

The following listing includes both the original main program using microfilm plotter and a main program TRYPEN which uses the pen plotter.

Reproduced from
best available copy.

```

      WTSF (5,10) MUMIN,MUMAX
      TNS = 10.0*MUMIN - 40.0
      TS (TNS,1,1) TNS = 1
      TMS = 10.0*MUMAX - 40.0
      TS (TMS,2,2) TMS = 200
      NY = TNS - TMS + 1
      NY = 12*NY
      DO 300 NP = 1, 2
        DEAN (2) AMAM
      DO 110 T = 1, NY
        X(T) = AMAM(TNS + T - 1)
      CONTINUE
      CALL ITMSEA (X,NX,SY,MTNY,MY,KMXY)
      CAS = SY/ELCOT(KMXY/10)
      SX = CAS*JY
      NCAS = MOC(KMXY,10)
      DO 250 NSC = 1, 7
        DEAN (2) SCSTAN
        TJ = 1
      DO 130 J = 1, 10
      DO 120 T = 1, NX
        Y(TJ) = SCSTAN(TNS + T - 1,J)
        TJ = TJ + 1
      CONTINUE
      CONTINUE
      CALL LOGSEA (Y,NV,SV,MTNY,MAYX,9)
      CALL STREAM (10)
      CALL ITMAXS (SV,0.0,VCOR,-NVI,SX,
1  90.0,XMTN,SY,CAS,NH,NCAS)
      CALL ITMAXS (0.0,0.0,XCOR,MVL,SY,
1  00.0,XMTN,SY,CAS,NH,-NCAS)
      CALL LOGAYS (SV,0.0,VCOR,MVL,SV,
1  180.0,MTNY,MAYX,1)
      CALL LOGAYS (SV,SV,VCOR,-MVL,SV,
1  180.0,MTNY,MAYX,0)
      CALL COIN (IEIY(SV/CAS - 0.0),CAS,SV)

```

TOST 370
 TOST 380
 TOST 390
 TOST 400
 TOST 410
 TOST 420
 TOST 430
 TOST 440
 TOST 450
 TOST 460
 TOST 470
 TOST 480
 TOST 490
 TOST 500
 TOST 510
 TOST 520
 TOST 530
 TOST 540
 TOST 550
 TOST 560
 TOST 570
 TOST 580
 TOST 590
 TOST 600
 TOST 610
 TOST 620
 TOST 630
 TOST 640
 TOST 650
 TOST 660
 TOST 670
 TOST 680
 TOST 690
 TOST 700
 TOST 710
 TOST 720

```

      CALL CPTC (MTNV + 1, MAXY, SY/ELCAT(MAXY - MTNV), SX)
150  DO 150 T = 1, NY
      Y(T) = SY - Y(T)
      CONTINUE
200  DO 200 J = 1, J2
      CALL STREAN (JOFAM(J))
      IJ = (J - 1)*NX + 1
      CALL MULTVE (V(TJ), Y, NY, SY, SX)
      CONTINUE
250  CALL FNAME (1.5, 1.5)
      CONTINUE
300  CONTINUE
      RETURN 2
400  CONTINUE
      CALL ENDELT
      CALL SECOND (SECA)
      SECC = SECA - SECA
      WRITE (NW, TENT) SECA, SECA, SECC
      STOP
      END

```

```

TCPT 730
TCPT 740
TCPT 750
TCPT 760
TCPT 770
TCPT 780
TCPT 790
TCPT 800
TCPT 810
TCPT 820
TCPT 830
TCPT 840
TCPT 850
TCPT 860
TCPT 870
TCPT 880
TCPT 890
TCPT 900
TCPT 910
TCPT 920

```

C

PROGRAM TRYPEN (TAPE2,TAPE5,OUTPUT,TAPE6=OUTPUT)

COMMON X,Y

DIMENSION IDENT(3)

DIMENSION X(1801),Y(1801)

DIMENSION XBCD(7),YBCD(7)

DIMENSION TFMT(6)

DATA IDENT /1GH FCWLER,10H 2105,10H SPEC A /

DATA TFMT /10H(/5X,5HSTA,10HRT,6X,3HEN,10HD,7X,5HIOT,

1 1JHAL,6X,5HI,10HMES/1X,3F1,5H0.3/)/

6 FORMAT (1X,I5)

8 FORMAT (1X,I2,1X,7A10)

10 FORMAT (1X,F9.3,1X,F9.3)

12 FORMAT (1P6E11.3)

16 FORMAT (1H1)

CALL SECOND (SECA)

NH = 6

REWIND 2

WRITE (6,16)

SY = 7.0

SX = 5.5

NX = 1801

NY = NX

NH = 2

CALL PLTID3 (IDENT,12J.0,12.0,1.0)

CALL PLOT (1.0,1.0,-3)

READ (5,8) NXL,XBCD

WRITE (6,8) NXL,XBCD

READ (5,8) NYL,YBCD

WRITE (6,8) NYL,YBCD

DO 25J NGRPH = 1, 2

READ (2,12) Y

10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
230
240
250
260
270
280
290
300
310
320

XX X=3.93.C	330
DO 110 I =1, 18(1	340
XX X = XX X + 2.0	350
X(I) = XX X	360
110 CONTINUE	370
CALL LINSCA (X,NX,SX,XMIN,DX,KONX)	380
GAP = SX/FLOAT(KONX/10)	390
GX = GAP*DX	400
N5AP = MOD(KONX,10)	410
CALL LOGSCA (Y,NY,SY,MINY,MAXY,9)	420
DO 200 J = 1, 1	430
CALL LINAXS (0.0,0.0,XBCD,-NXL,SX,	440
1 0.0,XMIN,GX,GAP,NH,NGAP)	450
CALL LINAXS (SX,SY,XBCD,-NXL,SX,	460
1 180.0,XMIN,GX,GAP,NH,-NGAP)	470
CALL LOGAXS (0.0,0.0,YBCD,NYL,SY,	480
1 90.0,MINY,MAXY,1)	490
CALL LOGAXS (SX,0.0,YBCD,-NYL,SY,	500
1 90.0,MINY,MAXY,0)	510
CALL GRID (MAXY - MINY - 1,SY/FLOAT(MAXY - MINY),SX)	520
CALL GRID (-IFIX(SX/GAP - 0.9),GAP,SY)	530
CALL NULINE (X,Y,NX,SX,SY)	540
CALL PLOT (9.0,0.0,-3)	550
200 CONTINUE	560
CALL LINAXS (0.0,0.0,XBCD,-NXL,SX,	570
1 0.0,XMIN,GX,GAP,NH,NGAP)	580
CALL LINAXS (SX,SY,XBCD,-NXL,SX,	590
1 180.0,XMIN,GX,GAP,NH,-NGAP)	600
CALL LOGAXS (0.0,0.0,YBCD,NYL,SY,	610
1 90.0,MINY,MAXY,1)	620
CALL LOGAXS (SX,0.0,YBCD,-NYL,SY,	630
1 90.0,MINY,MAXY,0)	640

C	CALL GRID (MAXY - MINY - 1,SY/FLOAT(MAXY - MINY),SX)	650
C	CALL GRID (-IFIX(SX/GAP - J.9),GAP,SY)	660
	DO 240 J = 1, 1	670
	CALL NULINE (X,Y,NX,SX,SY)	680
240	CONTINUE	690
	CALL PLOT (9.6,0.3,-3)	700
250	CONTINUE	710
300	CONTINUE	720
	REWIND 2	730
	CALL SECOND (SECB)	740
	SECC = SECB - SECA	750
	WRITE (NW,TFMT) SECA,SECB,SECC	760
	CALL ENDPLT	770
	STOP	780
	END	790

```

C
C
C
C
SUBROUTINE LINSKA (X,N,S,XMIN,DX,KON)

THE SCALING ALGORITHM GUARANTEES THAT THE PLOT WILL USE AT
LEAST SEVENTY PER CENT OF THE LENGTH OF A LINEAR AXIS.

    DIMENSION A(14),KA(14),KB(14),X(100)
    DATA A /1.0,1.2,1.5,1.8,2.0,2.4,3.0,4.0,5.0,6.0,7.5,
      1 9.0,10.0,12.0/
    DATA KA / 10,12,15,9,20,12,15,10,10,12,15,0,10,12 /
    DATA KB / 44,33,34,32,44,33,34,44,44,33,34,32,44,33 /
    XMX = X(1)
    XMN = XMV
    ADX = 0.0
    DO 110 I = 2, N
      XMX = AMAX1(XMX,X(I))
      XMN = AMIN1(XMN,X(I))
110 CONTINUE
    SX = XMX - XMN
    K = 0
120 CONTINUE
    IF (SX.GE. 0.99999) GO TO 130
    SX = 10.0*SX
    K = K + 1
    GO TO 120
130 CONTINUE
    IF (SX.LT. 10.0) GO TO 140
    SX = 0.1*SX
    K = K + 1
    GO TO 130
140 CONTINUE
    DO 150 I = 1, 14
      IF (SX.GT. 1.0005*A(I)) GO TO 150

```

ST = A(I)*10.0**K	330
DX = ST/LOAT(KA(I))	340
XMIN = XMN - AMOD(DX + AMOD(XMN,DX),DX)	350
DX = ST/S	360
KON = K3(I)	370
IF ((XMX - XMIN)/DX .LT. S*1.0005) GO TO 160	380
150 CONTINUE	390
160 CONTINUE	400
CO 220 I = 1, N	410
X(I) = (X(I) - XMIN)/DX	420
220 CONTINUE	430
300 CONTINUE	440
RETURN	450
END	460

```

C          SUBROUTINE LOGSCA (X,N,S,MIN,MAX,K)
C          IF K IS POSITIVE, K LOG CYCLES WILL BE PRODUCED.
C          IF K IS NEGATIVE, INPUT VALUE OF MIN WILL BE USED.
          DIMENSION X(100)
          MINSAV = MIN
          XX = ALOG10(ABS(X(1))) + 1.0E-99)
          X(1) = XX
          XMAX = XX
          XMIN = XX
          DO 110 I = 2, N
            XX = ALOG10(ABS(X(I))) + 1.0E-99)
            X(I) = XX
            XMAX = AMAX1(XMAX,XX)
            XMIN = AMIN1(XMIN,XX)
          110 CONTINUE
          MAX = XMAX
          MIN = XMIN
          IF (FLOAT(MAX) .LT. XMAX) MAX = MAX + 1
          IF (FLOAT(MIN) .GT. XMIN) MIN = MIN - 1
          IF (K .LT. 0) MIN = MINSAV
          IF (K .EQ. 0) GO TO 120
          MIN = MAX0(MIN, MAX - K)
          120 CONTINUE
          FAC = S / FLOAT(MAX - MIN)
          XMIN = MIN
          XLAST = -0.5
          GO 140 I = 1, N
          X(I) = (X(I) - XMIN)*FAC
          IF (X(I) .LT. -0.01) X(I) = -0.5
          IF (XLAST .GE. 0.0) GO TO 130
          XLAST = X(I)
          IF (I .EQ. 1) GO TO 140

```

```

      IF (X(I) .GE. 0.0) X(I-1) = -0.01
      GO TO 140
130  CONTINUE
      XLAST = X(I)
      IF (X(I) .LT. 0.0) X(I) = -0.01
140  CONTINUE
      RETURN
      END

```

330
 340
 350
 360
 370
 380
 390
 400

```

SUBROUTINE LINAXS (X,Y,BCD,NC,S,THETA,XMIN,DX,GAP,NH,NG)
DIMENSION BCD(8)
DATA W /10H X 10 /
NJ = IA3S(NG)
NSN = 1
IF (NC .LT. 0) NSN = -1
TH = THETA*0.017453294
SN = NSN
HC = NC*NSN
N = S/GAP + 0.5
S2 = 0.5*S
CTH = COS(TH)
STH = SIN(TH)
CFAC = CTH*GAP/FLOAT(NJ + 1)
SFAC = STH*GAP/FLOAT(NJ + 1)
NABS = IABS(NH)
ADJ = FLOAT(NABS)
IF (NABS .GT. 3) ADJ = 5.0
SADJ = ADJ*STH
CAJJ = ADJ*CTH
XA = X + 0.0875*SN*SADJ
YA = Y - 0.0875*SN*CAJJ
XD = X + 0.05*SN*SADJ
YD = Y - 0.05*SN*CAJJ
HEIGHT = 0.05*ADJ
CALL PLOT (XA,YA,3)
XB = X
YB = Y
DO 120 I = 1, N
DO 110 J = 1, NJ
CALL PLOT (XB,YB,2)
XC = XB + CFAC

```

Y3 = Y3 + SFAC	330
CALL PLOT (XC,YC,2)	340
X3 = XD + CFAC	350
Y3 = YD + SFAC	360
CALL PLOT (XD,YD,2)	370
X3 = XC	380
Y3 = YC	390
110 CONTINUE	400
CALL PLOT (XB,YB,2)	410
XC = XB + CFAC	420
YC = YB + SFAC	430
CALL PLOT (XC,YC,2)	440
XA = XA + GAP*CTH	450
YA = YA + GAP*STH	460
CALL PLOT (XA,YA,2)	470
X3 = XD + CFAC	480
YD = YD + SFAC	490
X3 = XC	500
Y3 = YC	510
120 CONTINUE	520
IF (NG .LE. 0) RETURN	530
A3SV = XMIN + DX*FLOAT(N)	540
IF (NH .LT. 0) GO TO 160	550
ADX = ABS(DX)	560
E = 3.0	570
130 CONTINUE	580
IF (ADX .EQ. 0.0) GO TO 150	590
IF (ADX .LT. 1.0) GO TO 140	600
ADX = ADX/10.0	610
E = E - 1.0	620
ABSV = 0.1*ABSV	630
GO TO 130	640

140	CONTINUE		650
	IF (ADX .GE. 0.1) GO TO 150		660
	ABSV = ABSV*10.0		670
	ADX = ADX*10.0		680
	E = E + 1.0		690
	GO TO 140		700
150	CONTINUE		710
	IF (DX .GE. 0.1) GO TO 160		720
	ADX = -ADX		730
160	CONTINUE		740
	XA = X3 - (0.1*SN - 0.025)*SADJ - 0.0964*CADJ		750
	YA = Y3 + (0.1*SN - 0.025)*CADJ - 0.0964*SADJ		760
170	CONTINUE		770
	N = N + 1		780
	CFAC = 0.0429*CADJ		790
	SFAC = 0.0429*SADJ		800
169	DO 200 I = 1, N		810
	IF (NH .LT. 0) GO TO 180		820
	CALL NUMBER (XA,YA,HEIGHT,ABSV,THETA,3)		830
	ABSV = ABSV - ADX		840
	GO TO 190		850
180	CONTINUE		860
	I80 = 1		870
	IF (ABS (ABSV) .GE. 10.0) I80 =		880
	1 IFIX(ALOG10(ABS(ABSV))) + 1.0E-9) + 1		890
	X3 = XA - CFAC*FLOAT(I80 - 1)		900
	Y3 = YA - SFAC*FLOAT(I80 - 1)		910
	CALL NUMBER (X3,Y3,HEIGHT,ABSV,THETA,3)		920
	ABSV = ABSV - DX		930
190	CONTINUE		940
	XA = XA - GAP*CTH		950
	YA = YA - GAP*STH		960

200	CONTINUE	970
	IF (NH .GE. 0) GO TO 210	980
	ANC = MC	990
	XA = X + (S2 - 0.035*ANC*ADJ)*CTH - (0.18*SN - 0.0335)*SADJ	1000
	YA = Y + (S2 - 0.035*ANC*ADJ)*STH + (0.18*SN - 0.0335)*CADJ	1010
	HEIGHT = 0.07*ADJ	1020
	CALL SYMBOL (XA,YA,HEIGHT,BCU,THETA,MC)	1030
	RETURN	1040
210	CONTINUE	1050
	TNC = MC + 7	1060
	XA = X + (S2 - 0.035*TNC*ADJ)*CTH - (0.1875*SN - 0.0375)*SADJ	1070
	YA = Y + (S2 - 0.035*TNC*ADJ)*STH + (0.1875*SN - 0.0375)*CADJ	1080
	HEIGHT = 0.07*ADJ	1090
	CALL SYMBOL (XA,YA,HEIGHT,BCU,THETA,MC)	1100
	IF (E.EQ. 0.0) RETURN	1110
	XA = XA + ((TNC - 6.0)*0.07*ADJ)*CTH	1120
	YA = YA + ((TNC - 6.0)*0.07*ADJ)*STH	1130
	CALL SYMBOL (XA,YA,HEIGHT,W,THETA,5)	1140
	IF (E - 1.0) 220,250,230	1150
220	CONTINUE	1160
	XA = XA + 0.35*CADJ - 0.035*SADJ	1170
	YA = YA + 0.35*SADJ + 0.035*CADJ	1180
	GO TO 240	1190
230	CONTINUE	1200
	XA = XA + 0.35*CADJ - 0.035*SADJ	1210
	YA = YA + 0.35*SADJ + 0.035*CADJ	1220
240	CONTINUE	1230
	HEIGHT = 0.05*ADJ	1240
	CALL NUMBER (XA,YA,HEIGHT,E,THETA,-1)	1250
250	CONTINUE	1260
	RETURN	1270
	END	1280

```

SUBROUTINE LOGAXS (X,Y,BCD,NC,S,THETA,MIN,MAX,NTEST)
DIMENSION BCD(8)
SN = 1.0
IF (NC .LT. 0) SN = -1.0
FAC = 1.0
TH = 0.017453294*THETA
CTH = COS(TH)
STH = SIN(TH)
CFAC = CTH*S/FLOAT(MAX - MIN)
SFAC = STH*S/FLOAT(MAX - MIN)
XL = J.1*SN*STH*FAC
YL = 0.1*SN*CTH*FAC
XM = 1.75*XL
YM = 1.75*YL
CALL PLOT (X + XM,Y - YM,3)
XA = X
YA = Y
N = 0
140 CONTINUE
P = 2.0
Q = 1.0
X3 = XA
Y3 = YA
150 CONTINUE
CALL PLOT (XB,YB,2)
PLOG = ALOG10(P/Q)
X3 = X3 + CFAC*PLOG
Y3 = Y3 + SFAC*PLOG
CALL PLOT (XB,YB,2)
IF (P .EQ. 10.0) GO TO 160
P = P + 1.0
Q = Q + 1.0

```

160	CALL PLOT (X3 + XL,Y3 - YL,2)	330
	GO TO 150	340
	CONTINUE	350
	CALL PLOT (X3 + X1,Y3 - Y1,2)	360
	N = N + 1	370
	XA = XA + CFAC	380
	YA = YA + SFAC	390
	IF (1 - MAX + MIN .LT. 0) GO TO 140	400
	IF (NTEST .EQ. 0) GO TO 300	410
	FAC = 0.7*FAC	420
	XP = MIN	430
	XA = X	440
	YA = Y	450
170	CONTINUE	460
	X3 = XA - ((0.325*SN - 0.1)*STH + 0.235675*CTH)*FAC	470
	Y3 = YA + ((0.325*SN - 0.1)*CTH - 0.235675*STH)*FAC	480
	RASE = 10.0	490
	IF (XP .NE. 0.0) GO TO 180	500
	X3 = X3 + 0.064175*CTH*FAC	510
	Y3 = Y3 + 0.064175*STH*FAC	520
	RASE = 1.0	530
180	CONTINUE	540
	CALL NUMBER (X3,Y3,0.15*FAC,BASE,THETA,-1)	550
	IF (XP .LT. 0.0) GO TO 200	560
	IF (XP .EQ. 0.0) GO TO 230	570
	IF (XP .EQ. 1.0) GO TO 230	580
190	CONTINUE	590
	XT = X3 + (0.3143*CTH - 0.1*STH)*FAC	600
	YT = Y3 + (0.3143*STH + 0.1*CTH)*FAC	610
	GO TO 220	620
200	CONTINUE	630
210	CONTINUE	640

```

220 XT = X3 + (0.3713*CTH - 0.125*STH)*FAC
    YT = Y3 + (0.3713*STH + 0.125*CTH)*FAC
    CONTINUE
230 CALL NUMBER (XT,YT,0.1*FAC,XP,THETA,-1)
    CONTINUE
    XA = XA + CFAC
    YA = YA + SFAC
    XP = XP + 1.0
    IF (XP - 1.0 - FLOAT(14X) .LT. 0.0) GO TO 170
    OC = FLOAT(NC)*SN
    T = S/FAC
    X3 = X + ((T - OC*0.20 - 0.05725)*J.5*CTH -
1      (.06*SN - 0.1)*STH)*FAC
    Y3 = Y + ((T - OC*0.20 - 0.05725)*0.5*STH +
1      (.06*SN - 0.1)*CTH)*FAC
    ND = OC
    CALL SYMBOL (XB,Y3,0.2*FAC,RCD,THETA,ND)
300 CONTINUE
    RETURN
    END

```

650
660
670
680
690
700
710
720
730
740
750
760
770
780
790
800
810
820
830
840

```

SUBROUTINE GRID (NL,SPACE,S)
  NI = IABS(NL)
  AX = 0.0
  AY = 0.0
  IF (SPACE.EQ. 0.0) GO TO 200
  IF (NL.EQ. 0) GO TO 200
  IF (NL.GT. 0) GO TO 120
  BX = 0.0
  BY = S
  DX = ABS(SPACE)
  DY = 0.0
  GO TO 130
120 CONTINUE
  BX = S
  BY = 0.0
  DX = 0.0
  DY = ABS(SPACE)
130 CONTINUE
  IT = 0
  DO 150 I = 1, NI
    AX = AX + DX
    AY = AY + DY
    BX = BX + DX
    BY = BY + DY
    IT = 1 - IT
    IF (IT.LT. 0) GO TO 200
    IF (IT.GT. 0) GO TO 140
    CALL PLOT (BX,BY,3)
    CALL PLOT (AX,AY,2)
    GO TO 150
140 CONTINUE
    CALL PLOT (AX,AY,3)

```

330
340
350
360
370

CALL PLOT (BX, BY, 2)
CONTINUE
CONTINUE
RETURN
END

150
200


```

SUBROUTINE NULINE (X,Y,N,SX,SY)
DIMENSION X(100),Y(100)
DL = 0.1
SXA = SX + DL
SYA = SY + DL
XA = X(1)
YA = Y(1)
IPNA = 2
IF (XA .LT. -DL) IPNA = 3
IF (XA .GT. SXA) IPNA = 3
IF (YA .LT. -DL) IPNA = 3
IF (YA .GT. SYA) IPNA = 3
CALL PLOT (XA,YA,3)
CO 150 I = 2, N
IPNB = IPNA
XA = X(I)
YA = Y(I)
IPNA = 2
IF (XA .LT. -DL) IPNA = 3
IF (XA .GT. SXA) IPNA = 3
IF (YA .LT. -DL) IPNA = 3
IF (YA .GT. SYA) IPNA = 3
IPN = 2
IF (IPNA + IPNB .NE. 4) IPN = 3
CALL PLOT (XA,YA,IPN)
150 CONTINUE
RETURN
END

```

10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
230
240
250
260
270
280

Program BCKGND (BGND)

Purpose: The main program BCKGND (short for BACKGROUND) serves primarily to control the operation of subroutines which compute vibrational populations and radiative rates. BCKGND reads and checks the input data, and transfers control to Subroutine BANRAD which computes vibrational populations, local optical thicknesses and volume radiances for all included bands of a single molecular species. When control is returned, BCKGND computes and outputs integrated band radiances for limb viewing (exoatmospheric) and seven endoatmospheric viewing angles at selected tangent heights or endoatmospheric altitudes.

Program Flow: The initial step in operation of BCKGND is the reading of all input data. The number IGAS of molecular species including total number density is read in. Then in the DO range ending with statement 170, the following operations are performed. The title card, containing alphanumeric identification, an index check number and maximum altitude considered for the species is read in and its check number checked against the index of the DO range. If the check succeeds, altitude and number densities are read into arrays ALT and STORE until an altitude corresponding to the maximum altitude is found. When this altitude is found, the logarithm of input number densities is formed in the DO range ending with statement 130 and control is passed to Subroutine INTERP which interpolates to form values at 1 km intervals up to 160 km and at 5 km intervals at higher altitudes. The interpolated values are converted

to number densities in the DO range ending with statement 160. In the DO range ending with statement 175, total atmosphere number densities are stored in array TOTDEN. Temperature data are then read in similarly in the DO range ending with statement 245 and interpolated values found by Subroutine INTERP. The complete set of number densities and temperatures is then pointed out. Next, vibrational level and band constants are read in for each species in the DO range ending with statement 331. The first card for each species contains an alphanumeric identification, number of vibrational levels NLEV, number of bands NBAN, molecular mass AMAS, and two vibrational energy transfer coefficients DEXT and DEXB. The alphabetic code is checked and if it is a valid code stored in array DATATY, these constants are transferred to the appropriate arrays. In the DO range ending with statement 313, constants for each vibrational level are read in, and card sequence numbers checked. In the DO range ending with statement 316, constants for each band are read in and card sequence numbers checked. For CO₂ and H₂O, tabular values of temperatures and associated vibrational energy exchange coefficients are read before the vibrational level and molecular band data.

The computation of molecular band radiances then proceeds in the following manner. The outer DO range index NLTE and ending with statement 900 controls the factors considered in a complete set of calculations for any of five possible sets. The corresponding DO statement may be varied depending on what factors are desired. See the description of Subroutine BANRAD for the effect

of different values of the index NLTE. Each cycle through the nested DO range with Index I and ending with statement 750 results in the computation of band radiance values for a single molecule. Action within this DO range is as follows.

Subroutine BANRAD is called and returns volume emission radiance values in array RAD and local optical thickness values in array TAU. Then for each band, line of sight band radiances are computed in the DO range ending with statement 840. Within this DO range, the value of NLTE is examined and appropriate headings are printed. Then trapezoidal rule integration is performed to determine the radiance arising along each of the eight lines of sight, including the modification necessary for the effects of optical thickness along the line of sight. The DO range ending with statement 830 controls the integration for each tangent height and endoatmospheric viewing level. In the current version, radiance values are computed at 5 km intervals of tangent height up to 150 km and at 25 km intervals above this level. The integration of radiance values is performed for each endoatmospheric viewing level in the DO range ending with statement 810. The integration begins at the viewing altitude. At each point on the line of sight, the contribution of the local volume emission rate to that received at the viewing point is computed by Subroutine SMI, which takes into account the effects of optical thickness between the emitting point and the viewing point. The equivalent integration for the limb viewing case is

performed in the DO ranges ending with statements 815 and 818. Upon completion of the integration for each tangent height and endoatmospheric viewing level, band radiances for that level are punched and printed. This punched output, together with that produced by Subroutine BANRAD, is used as input data to the special radiance program SPECTRA.

Tables V-2 through V-4 list the molecular bands in the program. These are followed by a sample set of input data and the program listing.

Table V-2
Water Vapor Band Data

Vibrational Transition		Band Center	Band Strength	Solar Flux
<u>Upper State</u>	<u>Lower State</u>	<u>Wavelength (μm)</u>	<u>at 296 K ($\text{mol}^{-1} \text{ cm}^2 \text{ cm}^{-1}$)</u>	<u>Band Center ($\text{photons cm}^{-2} \mu\text{m}^{-1}$)</u>
010	000	6.27	$1.06(-17)^*$	5.60(15)
020	000	3.17	$6.58(-20)$	3.50(16)
100	000	2.73	$3.62(-19)$	5.10(16)
001	000	2.66	$7.99(-18)$	5.40(16)
020	010	6.42	$8.61(-21)$	5.70(15)
100	010	4.85	$8.90(-23)$	1.20(16)
001	101	4.63	$4.90(-22)$	1.50(16)
030	010	3.26	$7.99(-23)$	3.30(16)
110	010	2.75	$1.50(-22)$	5.00(16)
011	010	2.68	$3.30(-21)$	5.40(16)
030	020	6.60	$7.00(-24)$	4.90(15)
030	000	2.14	$2.00(-22)$	9.30(16)
110	000	1.91	$1.83(-20)$	1.20(17)
011	000	1.88	$9.16(-19)$	1.25(17)

* Number in parentheses is power of ten.

Table V-3
Carbon Dioxide Band Data

Vibrational Transition		Band Center	Band Strength	Solar Flux
Upper State	Lower State	Wavelength (μm)	at 296 K ($\text{mol}^{-1} \text{cm}^2 \text{cm}^{-1}$)	Band Center (photons $\text{cm}^{-2} \mu\text{m}^{-1}$)
01101	00001	14.98	8.26 (-18)	4.60 (14)
10002	01101	16.18	1.44 (-19)	3.70 (14)
02201	01101	14.98	6.49 (-19)	4.60 (14)
11102	10002	15.45	2.22 (-20)	4.20 (14)
1102	02201	16.74	5.21 (-21)	3.35 (14)
03301	02201	14.97	3.82 (-20)	4.60 (14)
10001	01101	13.87	1.85 (-19)	5.80 (14)
00011	10001	10.41	4.91 (-22)	1.31 (15)
00011	00001	4.62	9.60 (-17)	1.60 (16)

Table V-4
Ozone Band Data

Vibrational Transition		Band Center	Solar Flux	
<u>Upper State</u>	<u>Lower State</u>	<u>Wavelength (μm)</u>	<u>Band Strength, 296 K ($\text{mol}^{-1} \text{ cm}^2 \text{ cm}^{-1}$)</u>	<u>(photons $\text{cm}^{-2} \mu\text{m}^{-1}$)</u>
010	000	14.27	$4.13(-19)^*$	5.30(14)
001	000	9.60	$1.29(-17)$	1.70(15)
100	000	9.06	$3.47(-19)$	1.90(15)
101	000	4.74	$1.33(-18)$	1.20(16)
111	000	3.59	$2.32(-20)$	2.50(16)
003	000	3.29	$1.10(-19)$	3.20(16)
101	100	9.92	$9.49(-21)$	1.50(15)
011	010	9.79	$4.23(-19)$	1.60(15)
002	001	9.74	$1.62(-19)$	1.60(15)
003	002	10.29	$1.66(-21)$	1.40(14)
011	000	5.81	$3.10(-20)$	6.90(15)

* Number in parentheses is power of ten.

LINE	TIME	WAVELENGTH	FLUX	WAVELENGTH	FLUX	WAVELENGTH	FLUX
11	3.7270E+03	1.6505E+06					
201	11	1.2500E+02	9.7000E+15	3.3000E+15			
301	11	2.4100E+00	5.4000E+16	1.5900E+13			
302	11	3.1500E+02	9.4000E+15	3.0000E+15			
NITROUS OXIDE - N2O							
11	3.0000E+00	4.1001E-01					
21	5.8800E+02	4.0000E-01					
31	1.1730E+03	4.0000E-01					
41	1.7580E+03	4.0000E-01					
51	2.3380E+03	4.0000E-01					
11	1	2.2235E+03	4.0000E-01				
11	1.2850E+03	4.0000E-01					
201	12	3.3000E+01	3.4000E+14	2.5000E+16			
701	11	2.6000E+02	3.0000E+15	1.0000E+16			
601	11	1.8560E+03	1.6000E+16	1.3000E+14			
OZONE PRE-DAWN - O3							
11	0.0000E+00	5.0000E-02					
11	7.0000E+02	5.0000E-02					
11	1.6420E+03	5.0000E-02					
11	1.1032E+03	5.0000E-02					
11	1.7220E+03	5.0000E-02					
11	2.0692E+03	5.0000E-02					
11	2.4100E+03	5.0000E-02					
11	2.7852E+03	5.0000E-02					
11	3.0412E+03	5.0000E-02					
201	11	4.1300E-19	5.3000E+14				
301	11	1.2900E-17	1.7000E+15				
401	11	3.4700E-19	1.9000E+15				
701	11	1.3300E-18	1.2000E+16				
801	11	2.3200E-20	2.5000E+16				
901	11	1.4000E-19	3.2000E+15				
704	11	9.4900E-21	1.5000E+15				
502	11	4.2300E-19	1.6000E+15				
603	11	1.6200E-19	1.6000E+15				
905	11	1.6500E-21	1.4000E+14				
201	11	3.1000E-20	6.0000E+15				
OZONE NOON - O3							
11	0.0000E+00	3.0000E-01					
11	2	1.0400E+03	3.0000E-01				
201	11	3.6000E+02	1.6000E+15	2.3000E+16			


```

PROGRAM BGND (INPUT, OUTPUT, PUNCH, TAPE1, TAPE2, TAPE3,
1 TAPE4=PUNCH, TAPE5=INPUT, TAPE6=OUTPUT)
2
3 DIMENSION XID(25,4), XIDT(4), ALT(30), STORE(30), IALT(25)
4 DIMENSION DATATY(25), CDEXT(25), CDEX8(25), NLEVE-(25), NBAND(25)
5 DIMENSION LSC(25,25), LCC(25,25), RCM(25,25), BV(25,25), AMASS(25)
6 DIMENSION ZANG(7), STAU(7), SRAD(8), RDN(8), RATIO(8)
7 DIMENSION LBC(25,25), LBU(25,25), STR(25,25), SFLJX(25,25), TFLUX(25,
8 125,3)
9 DIMENSION CO2(18,2), WATVA(18,2)
100 REAL LA1DA
110 COMMON /VBRCOM/ I,CO2,WATVA,CDEXT,CDEX8
120 COMMON /TEQCOM/ NLTE
130 COMMON/KCEM/KCEM
140 COMMON/INOUT/NR,NP,NW
150 COMMON CONC(201,10),TAU(201,25),RAD(201,25),T(211),LAMDA(25),
160 ITOTDEN(201)
170 DATA(7,NG(I),I=1,7)/0.0,20.0,40.0,60.0,70.0,80.0,90.0/
180 DATA(DATATY(I),I=1,25)/8HMETHANE,8HCARBON D,3HWATER VA,8HNITRIC O
190 1,8HNITROUS,8HOZONE PR,8HOZONE NO,18*8H
200 KCHEM = 1
210 NR = 5
220 NP = 3
230 NTX = 6
240 NW = 6
250 REWIND 1
260 REWIND 2
270 10 FOPMAT (I2)
280 20 READ(NR,10) IGAS
290 20 FOPMAT(1H1,22HNUMBER OF GAS PROFILES, I3)
300 WRITE(NW,20) IGAS
310 IGAS=IGAS+1
320 DO 170 J=1,IGAS

```



```

30 FORMAT (4A6,I3,F7.0)
READ(N2,30)(XID(J,K), K=1,4), ICHK,ALTM
IF(J.EQ.ICHK) GO TO 50
40 FORMAT (7HID CARD, A6, 20HOUT OF ORDER FOR GAS, I3)
WRITE(NW,40)(XID(J,K),K=1,4), J
50 DO 105 K=1,6
K1=(K-1)*5+1
K2=K1+4
60 FORMAT (5(F5.0,E8.1,2X),I2,I3)
READ(N2,60)(ALT(L),STORE(L),L=K1,K2), ICHK, K2+K
IF(ICHK.EQ.J) GO TO 80
70 FORMAT(30HDATA CARD OUT OF ORDER FOR GAS,I3, 5X, 8HCARD NO., I3)
IFIVE = 5
WRITE (NW,70) J,IFIVE
80 IF(KCHK.EQ.K) GO TO 90
WRITE (NW,70) J,K
90 DO 100 L=K1,K2
IF(ALT(L).LT.ALTM) GO TO 39
KSET=L
GO TO 120
99 CONTINUE
100 CONTINUE
105 CONTINUE
110 FORMAT(42HMAX ALT. NOT FOUND ON DATA CARDS - GAS NO., I3)
WRITE(NW,110) J
120 DO 130 L=1,KSET
130 STORE(L)=ALOG(STORE(L))
IF(ALTM.GT.150.) GO TO 140
IALF(J)=ALTM-59.
GO TO 150
140 IALF(J)=91.+(ALTM-150.)/5.
150 CALL INTERP(ALT,STORE,KSET,1,J)

```

```

L1=IALT(J)
DO 160 L=1,L1
160 CONC(L,J)=EXP(CONC(L,J))
170 CONTINUE
DO 175 J=1,201
175 TOTDEN(J)=CONC(J,IGAS)
READ(NP,30) (XIDT(K),K = 1,4), ICHK, KCHK
IF(ICHK.EQ.1) GO TO 190
180 FORMAT(7HID CARD, 4A6,26HOUT OF ORDER FOR TEMP DATA)
WRITE(NW,180) (XIDT(K),K=1,4)
190 DO 245 K=1,6
K1=(K-1)*5+1
K2=K1+1
READ(NP,60) (ALT(L),STORE(L),L=K1,K2), ICHK, KCHK
IF(ICHK.EQ.1) GO TO 210
200 FORMAT(31HTEMP DATA CARD OUT OF ORDER NO.,I3)
WRITE(NW,200) K
210 IF(KCHK.EQ.K) GO TO 230
220 WRITE(NW,210) K
230 DO 240 L=K1,K2
IF(ALT(L).LT.ALTM) GO TO 240
KSET=L
GO TO 250
240 CONTINUE
245 CONTINUE
250 FORMAT(37HMAX ALT. NOT FOUND ON TEMP DATA CARDS)
WRITE(NW,250)
260 CAL=INTERP(ALT,STORE,KSET,2,1)
261 FORMAT(1X,I5,1P9E12.4)
WRITE(NW,261) (J,(CONC(J,I),I=1,IGAS), T(J),J = 1,201)
IGAS=IGAS-1
DO 331 II=1,IGAS

```

```

310 READ(NR,310)TYPE,NLEV ,NBAN ,AMAS ,DEXT,DEXB
    FORMAT (A8,22X,I2,3X,I2,3X,F6.2,4X,2(E12.4,3X))
    DO 311 J=1,25
    IF (TYPE.EQ.DATATY(J)) GO TO 312
311 CONTINUE
    WRITE(NW,370)
370 FORMAT(36HTHE GAS IS NOT LISTED IN THE PROGRAM)
    STOP 1
C 312 NSP=J
    NLEVEL(NSP)=NLEV
    NBAND(NSP)=NBAN
    AMASS(NSP)=AMAS
    CDEXT(NSP)=DEXT
    CDEXR(NSP)=DEXB
    IF(NSP.EQ.2)READ(NR,320) (C02(I,1),C02(I,2),I=1,18)
320 FORMAT (6(F5.2,F8.2))
    IF(NSP.EQ.3)READ(NR,320) (WATVA(I,1),WATVA(I,2),I=1,18)
    ILEV=7
    DO 313 IJ=1,NLEV
    ILEV=ILEV+1
    READ(NR,330)LSC(NSP,IJ),LCC(NSP,IJ),RCM(NSP,IJ),BV(NSP,IJ),JGAS,
1JLEVEL
330 FORMAT (2I6,2E12.4,36X,2I3)
    IF(NSP.EQ.JGAS) GO TO 314
    WRITE(NW,340) NSP
340 FORMAT(64HTHE CODE ON THE DATA DOES NOT AGREE WITH THE FIRST CARD
1WHICH IS,I3)
C 314 IF(ILEV.EQ.JLEVEL) GO TO 313
    WRITE (NW,350) NSP
350 FORMAT(42HTHERE IS A CARD OUT OF SEQUENCE IN SAS NO.,I3)
C 315 STOP 3

```

```

313 CONTINUE
ILEVL=0
DO 316 IJ=1,NBAN
ILEVL=ILEVL+1
READ(NP,360)LBC(NSP,IJ),LBU(NSP,IJ),STR(NSP,IJ),SFLUX(IJ,NSP),
1(TFLUX(IJ,NSP,J),J=1,3),JGAS,JLEVEL
STR(NSP,IJ) = 2.4793E+19*STR(NSP,IJ)
360 FORMAT (2I6,1P5E12.4,2I3)
IF(NSP.EQ.JGAS) GO TO 322
WRITE (NW,340) NSP
C STOP 4
322 IF(ILEVL.EQ.JLEVEL) GO TO 316
WRITE (NW,350) NSP
C STOP 5
316 CONTINUE
331 CONTINUE
WRITE (NP,378) T
378 FORMAT (1P6E12.4)
DO 300 NLTE = 3, 4
NSPTOT = 4
WRITE (NP,360) NSPTOT
DO 950 I = 2, 7
IF ((I.EQ. 6) .AND. (NLTE.EQ. 4)) GO TO 850
IF ((I.EQ. 7) .AND. (NLTE.EQ. 3)) GO TO 850
IF (I.EQ. 5) GO TO 850
WRITE (NP,360) I
WRITE (NP,360) NLEVEL(I),NBAND(I),AMASS(I)
NLEV = NLEVEL(I)
NBAND = NBAND(I)
DO 381 IJ = 1, NLEV
WRITE (NP,360) LSC(I,IJ),LCC(I,IJ),RCM(I,IJ),BV(I,IJ)
381 CONTINUE

```

1290
1300
1310
1320
1330
1340
1350
1360
1370
1380
1390
1400
1410
1420
1430
1440
1450
1460
1470
1480
1490
1500
1510
1520
1530
1540
1550
1560
1570
1580
1590
1600

```

DO 342 IJ = 1, NBND
  WRITE (NP,360) LBC(I,IJ),LBU(I,IJ),STR(I,IJ)
382 CONTINUE
  JALT = (IALT(I) - 1)/5
  WRITE (NP,360) IALT(I),JALT
  CALL BANRAD (NLEVEL(I),NBAND(I),IALT(I),CDEX(I),CDEX8(I),
1    AMASS(I),LSC(I,1),LCC(I,1),LBC(I,1),LBU(I,1),BV(I,1),STR(I,1),
2    RCM(I,1),CONC(1,I),SFLUX(1,I),TFUX(1,I,1))
  KK=IALT(I)
  JSET=N3AND(I)
DO 340 J=1,JSET
700 FORMAT('H1,4A6,8HBAND NO.,I3,5X,7HLAMDA =,F6.2,7HMICRO M,4X,4A6//')
  WRITE(NW,700)(XID(I,K),K=1,4),J,LAMDA(J),(XIDJ(K),K=1,4)
  IF (NLTE .GT. 1) GO TO 707
704 FORMAT(40H ASSUMES LOCAL THERMODYNAMIC EQUILIBRIUM/)
705 WRITE(NW,704)
  GO TO 715
706 FORMAT(28H LACK OF THERMAL EQUILIBRIUM ,I6/)
707 WRITE (NW,706) NLTE
710 FORMAT(118H EXOATMOSPHERIC VIEWING $$ - - - - - E N D
1 0 A T M O S P H E R I C V I E W I N G - - - - -)
715 WRITE (NW,710)
720 FORMAT(118H TAN HT LIMB BAND RAD $$ ALTD - - - - - BAND RAD
1 ANCE AS A FUNCTION OF ZENITH ANGLE (WATTS/CM2-STER)- - - - -)
  WRITE (NW,720)
730 FORMAT(118H (KM) (WATTS/CM2-STER) $$ (KM) J DEG - UP 20 DEG
1 40 DEG 60 DEG 70 DEG 80 DEG 90 DEG-HORZ )
  WRITE (NW,730)
740 FORMAT (F5.0,1PE14.4,0PF12.0,1X,1P7E12.4)
  KSET=JALT(I)-1
DO 370 K=1,KSET,5
  IF (.GT.91) GO TO 750

```

```

HT=K+50
GO TO 750
750 HT=150+(K-91)*5
760 D1=HT+6371.
DO 810 L=1,7
M1=K+1
PHI=7ANG(L)*.017453292
SAVTAU=0.0
STAU(L)=0.0
SRAD(L)=0.0
RANG=0.0
MSEI=IALT(I)
DO 790 I=M1,MSET
IF (M.GT.91) GO TO 770
D2=M+50+6371
GO TO 780
770 D2=150+(M-91)*5+6371
780 ANG=ASIN(SIN(PHI)*D1/D2)
DS=SQRT(D1*D1+D2*D2-2.*D1*D2*COS(PHI-ANG))
DELS=(DS-RANG)*1.0E+05
RANG=DS
STAU(L)=STAU(L)+DELS*(0.5*(TAU(M,J)+TAU(M-1,J)))
SRAD(L)=SRAD(L)+DELS*0.5*(RAD(M,J)*SM1(MOD(LBJ(I,J),10),STAU(L))
1+RAD(M-1,J)*SM1(MOD(LBU(I,J),10),SAVTAU))
SAVTAU=STAU(L)
790 CONTINUE
810 CONTINUE
SAVTAU=0.0
STAU(7)=0.0
VRANG = 0.0
SRAD(9)=0.0
MSEI=IALT(I)

```

```

00 815 M=K,MSET
NSHEL5 = 2*(MSET-K) + 1
L=MSET-M+K
IF (L.GT.91) GO TO 811
D2=_.+59+6371
GO TO 812
811 D2=150+(L-91)*5+6371
812 DS=SQR(02*D2-D1*D1)
D3 = D2 - 6371.
IF (L.LT.MSET) GO TO 813
RANG=DS
SAVF1=1.0
GO TO 815
813 DELS=(RANG-DS)*1.0E+05
VRANG = VRANG + DELS
RANG=DS
STAJ(7)=STAU(7)+DELS*(0.5*(TAU(L,J)+TAU(L+1,J)))
SAVF2=SAV1(MOD(LBU(I,J),10),STAU(7))
SRAD(8)=SRAD(8)+DELS*(0.5*(RAD(L,J)*SAVF2+RAD(L+1,J)*SAVF1))
819 SAVF1=SAVF2
815 CONTINUE
M1=<+1
RANG=0.0
MSEF=IAIT(I)
00 818 M=M1,MSET
IF (M.GT.91) GO TO 816
D2=M+50+6371
GO TO 817
816 D2=150+(M-91)*5+6371
817 DS=SQR(02*D2-D1*D1)
D3 = D2 - 6371.
DELS=(DS-PRANG)*1.0E+05

```



```

VRANG = VRANG + DELS
RANG=NS
STAU(7)=STAU(7)+DELS*(0.5*(TAU(M,J)+TAU(M-1,J)))
SAVT2=SM1(MOD(LBU(I,J),10),STAU(7))
SRAD(8)=SRAD(8)+DELS*(0.5*(RAD(M,J)*SAVT2+RAD(M-1,J)*SAVT1))
820 SAVT1=SAVT2
818 CONTINUE
WRITE(NP,4444) HT,SRAD(8),SRAD(1),SRAD(7)
4444 FORMAT (F6.1,1P3E17.4)
WRITE(NP,740) HT,SRAD(8), HT,(SRAD(M), M= 1,7)
830 CONTINUE
840 CONTINUE
850 CONTINUE
900 CONTINUE
REWIND 1
REWIND 2
STOP 77
END
2570
2580
2590
2600
2610
2620
2630
2640
2650
2660
2670
2680
2690
2700
2710
2720
2730
2740

```

```

SURROUTINE INTERP(ALT,STORE,KSET,MODE,I)
DIMENSION ALT(30),STORE(30)
COMMON CONC(201,10),TAU(201,25),RAD(201,25),T(201),LAMDA(25),
1TOTDEN(201)
J=1
A=50.
8 DO 120 K=1,KSET
10 IF(A-A.T(K))80,20,20
20 GO TO (30,40),MODE
30 CONC(J,I)=STORE(K)
GO TO 50
40 T(J)=STORE(K)
50 IF(K.LT.KSET) GO TO 60
RETURN
60 IF(J.GE.91) GO TO 70
A=A+1.
GO TO 110
70 A=A+5.
GO TO 110
80 FR=(A-ALT(K-1))/(ALT(K)-ALT(K-1))
GO TO (90,100),MODE
90 CONC(J,I)=STORE(K-1)+FR*(STORE(K)-STORE(K-1))
J=J+1
IF(J.GT.91) GO TO 92
A=A+1.
GO TO 10
92 A=A+5.
GO TO 10
100 T(J)=STORE(K-1)+FR*(STORE(K)-STORE(K-1))
GO TO 91
110 J=J+1
120 CONTINUE

```

10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
230
240
250
260
270
280
290
300
310
320

330
340

RETURN
END

Subroutine BANRAD

Purpose: BANRAD computes the population of vibrational levels of infrared active species, including the effects of collisional excitation; absorption of radiation from the lower atmosphere, sun and molecules radiating at high altitude. The values returned to the main program are volume radiance and unit optical thickness at each altitude for each band included in the computation.

Method: Subroutine BANRAD computes the population of vibrational levels of infrared active species, including the effects of collisional excitation and absorption radiation from the lower atmosphere, sun and molecules radiating at high altitude. The values returned to the main program are volume radiance and unit optical thickness at each altitude for each band included in the computation.

The collisional processes which are assumed to effect the vibrational state of a molecule are (1) translational-vibrational (T-V) interactions in which translation energy is transformed into vibrational energy or vice-versa during a collision, (2) intermolecular vibrational exchange (V-V) in which a molecule of one species exchanges a quantum of vibrational energy with a molecule of another species, and (3) intramolecular vibrational exchange in polyatomic molecules in which a collision transfers the energy in one mode of vibration into another mode within the same molecule.

When a molecule in the ground state collides with another molecule there is a finite probability P_{TV} that a portion of the relative translational energy will be transformed to vibrational energy if the translational energy is equal to or exceeds the vibrational energy. Similarly, if the molecule is in an excited vibrational state, there is a finite probability P_{VT} that the vibrational energy will be converted to relative translational energy during the collision. For a Boltzmann distribution of translational energies at a given temperature

$$P_{TV} = P_{VT} \frac{g_u}{g_l} \exp \left(- \frac{hc}{\lambda_o kT} \right)$$

where g_u and g_l are the statistical weights of the upper and lower vibrational levels, h is Planck's constant (6.6256×10^{-27} erg-sec), c is the velocity of light (2.9979×10^{10} cm/sec), k is the Boltzmann constant (1.38054×10^{-16} erg/K), T is absolute temperature (K) and λ_o is the wavelength (cm) corresponding to the energy difference of the two vibrational levels. Similar expressions hold for intermolecular and intramolecular V-V transfer.

The rate at which a vibrational level of a single molecule is excited (K_{TV}) or de-excited (K_{VT}) is given by the product of the collision frequency Z and the transition probability. The subroutine uses temperature dependent rate coefficients k_{TV} , k_{VT} , etc., such that if $[M]$ is the concentration of the collision partner, $K_{VT} = k_{VT}[M]$, etc.

The radiative processes which are assumed to affect the vibrational state of a molecule are (1) absorption of solar radiation, (2) absorption of radiation from the lower atmosphere, (3) absorption of radiation emitted by molecules in the upper atmosphere and (4) spontaneous emission at a rate $A_{u1}(\text{sec}^{-1})$, the Einstein A coefficient. Because absorbing molecules are present between each source of radiation and the molecule for which the vibrational state is to be computed, radiative transfer functions must be used to take into account the effects of absorption. The model assumes that individual lines have a Doppler (thermal velocity broadened) spectral contour.

At a given altitude, there will be N_1 molecules/cm³ in the ground vibrational state of a molecule and N_u molecules/cm³ in an upper state. Molecular nitrogen and oxygen are assumed to be the only collision partners effective in transfer of vibrational quanta, and their concentrations are used to determine total vibrational excitation rates K_{TV} , K_{VT} , etc. The treatment below refers to a two state molecule.

In unit volume, molecules in the ground state are excited to the upper state by:

- (1) Collisional T-V excitation at a rate $N_1 K_{TV}$
- (2) Collisional V-V excitation at a rate $N_1 K_{MV}$
(the subscript MV is used for excitation, VM for de-excitation, by transfer of vibrational quanta).

- (3) Absorption of solar flux at a rate $N_1 I_o G' M_1^b(k_s)$
where G' is molecular cross section for absorption of radiative flux
- (4) Absorption of lower atmospheric radiance at a rate $N_1 N_{\lambda, t} G' N_{12}^b(k_t)$
- (5) Absorption of radiance emitted at other levels of the atmosphere at a rate $N_1 \int N_{\lambda, D} G' N_{21}^b(k_D) dz$

Molecules in the upper state are de-excited by:

- (1) Collisional V-T de-excitation at a rate $N_u K_{VT}$
- (2) Collisional V-V de-excitation at a rate $N_u K_{VM}$
- (3) Spontaneous radiative de-excitation at a rate $N_u A_{u1}$

Excitation rates are assumed to balance de-excitation rates and the equation

$$\begin{aligned} \frac{dN_u}{dt} = & N_1 (k_{TV} + K_{MV} + I_o G' M_1^b(k_s) + N_{\lambda, t} G' N_{12}^b(k_t) \\ & + \int N_{\lambda, D} G' N_{21}^b(k_D) dZ - N_u (K_{VT} + K_{VM} + A_{u1}) = 0 \end{aligned}$$

is solved by iteration to determine N_u and N_1 at all altitudes.

Program
Flow:

The first step in the computation is determination of the thermal equilibrium populations of vibrational levels. This is performed in the DO range ending with statement 130. Each passage through this DO range computes populations for one altitude. Within this DO range are two others. The DO range ending with statement 110 computes the vibrational population of each level relative to the ground vibrational level, using the energies (wave-number) stored in WAVE and the statistical weights stored temporarily in real array VIBPOP. The sum of relative populations is stored in SUM. The final ground state population is then computed by dividing total concentration by SUM, and stored in real array GNDSTE. The DO range ending with statement 120 then computes the vibrational population of each level by multiplying total concentration by relative concentration divided by SUM.

The DO range ending with statement 135 selects the vibrational level which is coupled with the first excited nitrogen vibrational level.

The DO range ending with statement 160 computes the rate at which a single molecule in a given level is excited or de-excited by collisions at each altitude.

The outer DO range ending with statement 180 computes wavelengths (BNDLAM), Einstein A coefficients (EA), rates for absorption of radiation from the sun (GDOWN) and from the earth and lower atmosphere (GUP) and the G factor used in computing radiative transfer within the upper atmosphere (GFAC). The inner DO range ending

with Statement 180 computes the unit optical thicknesses for each band at each altitude using Function TAUMAX, and stores the result in array BNDTAU. In addition, it computes the volume radiances and stores them in array BNDRAD.

At this point, if NLTE is 1, computation for thermal equilibrium is complete and control is transferred to Statement 900. If NLTE is not 1, the computation for non-equilibrium is performed iteratively in the DO range ending with Statement 400. The DO range ending with Statement 190 computes various integrated optical thicknesses for each band. The DO range ending with Statement 182 computes the total thickness between each two altitudes in the vertical direction and stores the values in array TTH.

The DO range ending with Statement 184 (1) computes the optical thickness between the base altitude and each other altitude, storing the result in array TTUP and (2) computes the total optical thickness between the top altitude and each other altitude, storing the results in array TTDOWN. If the computation is not for daytime conditions, the DO range ending with Statement 186 sets the values in TTDOWN equal to 0.0, for efficiency in the later computations. If the computation is for the effects of collisional excitation only, the DO range ending with Statement 188 sets the values in TTUP equal to 0.0

The computation of vibrational populations now begins. Control is transferred to

Statement 210 if I is 1, CH₄

Statement 220 if I is 2, CO₂

Statement 230 if I is 3, H_2O

Statement 240 if I is 4, NO

Statement 250 if I is 5, N_2O

Statement 230 if I is 6, pre-dawn Ozone

Statement 230 if I is 7, noon Ozone

Following each of these statements is a DO range in which vibrational populations are computed. A discussion of two statements in the computation for CO_2 will illustrate the computational details. First, look at the statement in the DO range immediately following Statement 221 that begins VIBPOP(NZ, 8) = which computes the population of the first level of the ν_3 vibrational mode. This vibrational level is coupled to the nitrogen first vibrational level by collision, to the upward flux from the earth and lower atmosphere, to solar flux, and to lower vibrational levels by radiation. Excitation by absorption of radiation from within the upper atmosphere is neglected for this level. A ground state molecule is excited by collision with nitrogen at the rate VVNSIG(NZ) (collision exchange), by absorption of solar flux at a rate $GDOWN(9)*SM1(KB(9), TDOWN2(NZ))$ (equals $I_0 G'_1 M_1^b(k_s)$) and by absorption of flux from the earth and lower atmosphere at a rate $GUP(9)*SLM1(KB(9), TTUP2(NZ))$ (equals $N_{\lambda,t} G'_1 N_1^b(k_t)$). An excited molecule is de-excited by radiation at the rate EA(9) (other Einstein A coefficients are negligible), by vibrational exchange with nitrogen at a rate VVRSIG(NZ), and by transfer of vibrational energy to other modes within the CO_2 molecule at a rate VVDSIG(NZ). The vibrational population is then the ground state population times the ratio of excitation

and de-excitation rates. Second, look at the statement beginning POP2 = ..., which computes the vibrational population of level 2, the first excited level of the ν_2 vibrational mode. This level is excited from the ground state by collisional excitation at a rate TVS = TVSIG, by absorption of radiation from the lower atmosphere and earth at a rate GUP(1)*SLM1(KB(1), TTUP(NZ, 1)) (equals $N_{\lambda, t} G' N_1^b(k_t)$), by absorption of radiation from other points in the upper atmosphere in the 15.0 μ m fundamental band at a rate $2\pi * GFAC(1) * (XFER(VIBPOP(1, 2), TTH(1, 1), NZ, 1, 1, KB(1)) + XFER(VIBPOP(NZ, 2), TTH(NZ, 1), NALT, NZ, 2, KB(1))) * EA(1)$ (equals $\int N_{\lambda, D} G' N_2^b(k_D) dz$) and by absorption of solar radiation at the rate GDOWN(1)*SMI(KB(1), TTDOWN(NZ, 1)) (equals $I_o G' M_1(k_s)$). It is excited from levels 3, 4 and 7 by collisional excitation VTS and by radiation EA(2), EA(3) and EA(7). De-excitation occurs by radiation EA(1), and by collisional de-excitation to the ground state at a rate VTS = VTSIG(NZ), and by collisional excitation to higher states at a rate TVS. The approximate vibrational population is then the ratio of the sums of population rates times higher state populations divided by the sum of de-excitation rates for single molecule.

After each set of vibrational populations is completed, new values for volume band radiances are computed in the nested DO ranges ending with Statement 360.

After three iterations to compute vibrational populations control is returned to the main program.

Inputs: NLEVEL, NBAND, NALT, CDEXT, CDEXB, RM, LSC, LCC, I, LBC, LBU, BV, STR, WAVE, CONC, SFLUX, TFLUX, KCHEM, NR, NP, NW, NLTE, TEMP, BNDLAM, DENTOT, NBAND1.

Outputs: VIBPOP, BNDTAU, BNDRAD

Mnemonic Variables:

AA	intermediate factor in computing vibrational populations
AAA	quantity used in NO chemiluminescence calculation in original Subroutine BANRAD application; it has no effect at present
BNDL	wavelength of current interest (μm)
BNDLAM	wavelength array (μm)
BNDRAD	volume radiance
BNDTAU	unit optical thickness
BV	rotational constant (cm^{-1})
CDEXB	rate coefficient at 300 K for vibrational de-excitation of lowest NO vibrational level ($\text{cm}^3 \text{sec}^{-1}$)
CDEXT	rate coefficient at 300 K for vibrational exchange of NO with N_2 or O_2 for the most significant vibrational level ($\text{cm}^3 \text{sec}^{-1}$)
CHEML	currently inactive
CONC	array of NO concentrations (cm^{-3})
CO2	real array used to store reduced temperature value and rate coefficients to generate vibrational energy exchange rates for CO_2 : currently inactive
DENTOT	array of total number densities at altitude mesh (cm^{-3})

EA	array of Einstein A coefficients
FAC	used as temporary storage
FACTOR	temporary storage in computing vibrational exchange
GDOWN	real array in which are stored rates of absorption of solar radiation, $I_0 G'$ for each band
GFAC	real array in which are stored values of G' for each band
GNDSTE	real array in which are stored ground state vibrational populations, equivalenced to VIBPOP(1, 1)
GUP	real array in which are stored rates of absorption from the lower atmosphere, $2\pi N_{\lambda,t}^b G'$ for each band
I	index of species of interest (equals 4 for NO)
ITER	integer used as index in iterative computation of vibrational level population
IX	index for altitude level
JF	index for final vibrational level in a band transition
JI	index for initial vibrational level in a band transition
JL	integer used to compute JI, JF
JX	index for vibrational level
KB	integer array used to store band types
KBN	index of band type
KCHEM	chemiluminescence index; currently has no effect
KL	integer array storing level types
KLN	current level type
LBC	integer array containing information on which levels produce a band
LBU	integer array containing band type information
LCC	integer array containing vibrational level coupling go N_2 or O_2

LSC	integer array containing level type information
NALT	number of altitudes for which results are to be returned
NB	index for band number
NBAND	number of bands for this species
NBAND1	equal to NBAND
NBC	temporary storage index
NBX	temporary storage index
NF	temporary storage index
NI	temporary storage index
NL	level number index
NLEVEL	number of vibrational levels for this species
NLTE	integer variable used to indicate conditions of computation, 1 for local thermodynamic equilibrium, 2 for collisional excitation only, 3 for night conditions, 4 for noon conditions, 5 to include high vibrational temperature for nitrogen
NMIN	integer variable storing (NALT - 1)
NP	output device index
NR	input device index
NW	output device index
NY, NZ	index for altitude level
POP2, POP3, POP4, POP5, POP6, POP7, POP8	real variables used as temperature storage for vibrational populations
POWER	real array in which are stored conversion factors between emission rates in photons $\text{cm}^{-3} \text{sec}^{-1}$ and watts $\text{cm}^{-3} \text{ster}^{-1}$ for each band
RM	molecular mass for this molecule (g/mole)

SFLUX	array of solar flux values for each band
SNB	temporary storage of band strength ($\text{cm}^{-1}(\text{atm-cm})^{-1}$)
STR	array of band strength for each band ($\text{cm}^{-1}(\text{atm-cm})^{-1}$)
SUM	used to store partial sums
TDOWN2	real array equivalenced to TTDOWN(1, 9)
TEMP	array containing temperature profile (K)
TFLUX	array containing fluxes for lower altitudes for each band
TMP	temporary storage for temperature (K)
TNNV	nitrogen vibrational temperature (K)
TTDOWN	array storing values of total optical thickness from top of atmosphere for each band
TTH	array storing values of total optical thickness between adjacent altitudes for each band
TTUP	array storing values of total optical thickness from bottom of upper atmosphere for each band
TTUP2	array equivalenced to TTUP(9, 1)
TVS	used to store local value of TVSIG
TVSIG	array storing values of vibrational populations of each state for each altitude
VIBPOP	array storing values of vibrational populations of each state for each altitude
VTs	local value of VTSIG
VTSIG	array of vibrational de-excitation rates at each altitude
VVDSIG	array of estimated values of transfer of vibrational energy (downward)
VVNSIG	array of rates of transfer of vibrational energy from N_2 to this molecule
VVRSIG	array of rates of transfer of vibrational energy to N_2

VVUSIG	array of estimated values of rate of transfer of vibrational exchange (upward)
VVWAVE	difference between N ₂ vibrational energy and a molecular vibrational energy
WATVA	array storing reduced temperature values and rate coefficients to generate vibrational energy exchange rates for CO ₂
WAVE	array containing energy level of each band (cm ⁻¹)
XYM	temporary storage variables
XYMM	temporary storage variable
XYN	temporary storage variable

Non-Library Externals:

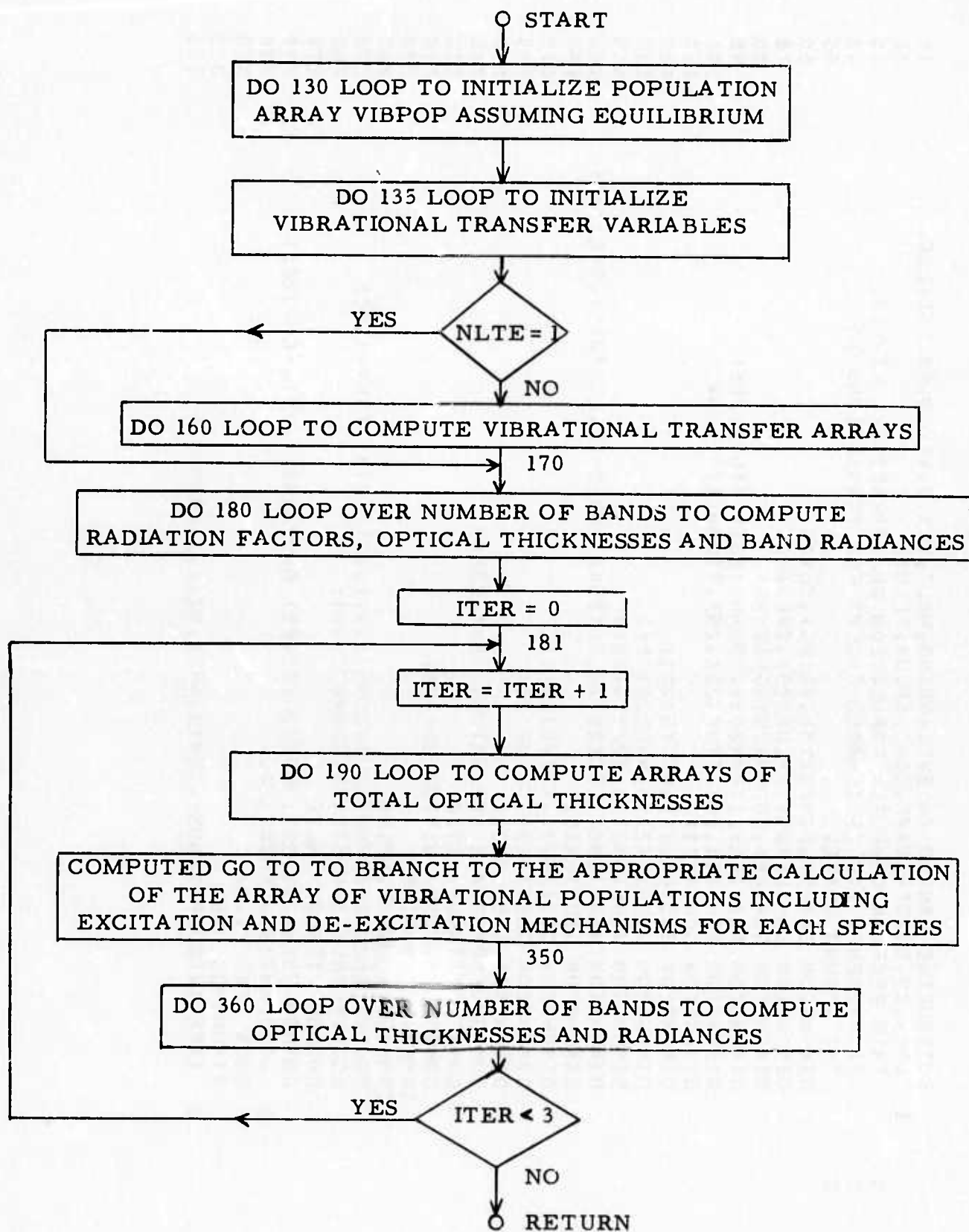
EVAL, SIMP, SLM1, SM1, TAUMAX, XFER

Called By:

BCKGND

FLOW CHART:

BANRAD



```

1  SUBROUTINE BANRAD (NLEVEL,NBAND,NALT,TEXCO,VEXCO,RM,LSC,LCC,
C   LBC,LBU,BV,STR,WAVE,CONC,SFLUX,TFLUX)
C   THIS SECTION COMPUTES POPULATION OF VIBRATIONAL LEVELS.
C   AT PRESENT, TAU IS IGNORED EXCEPT FOR TRANSITIONS TO
C   THE GROUND STATE.
    DIMENSION EA(25),POWER(25),KB(25),KL(25)
    DIMENSION EAHALF(25),TFLUX(25),SFLUX(25)
    DIMENSION GUP(25),GDOWN(25),GFAC(25)
    DIMENSION TR2(201),TTH2(201),TDOWN2(201),TTUP2(201)
    DIMENSION TTH(201,25),TTUP(201,25),TDOWN(201,25)
    DIMENSION CONC(201)
    DIMENSION TVSIG(201),VTSIG(201)
    DIMENSION VVUSIG(201),VVDSIG(201)
    DIMENSION VVMSIG(201),VVRSIG(201)
    DIMENSION WAVE(250),LSC(250),LCC(250),LBC(250),LBU(250),STR(250)
    DIMENSION GNDSTE(201)
    DIMENSION C02(18,2),WATVA(18,2)
    DIMENSION CDEXT(25),COEXR(25)
    DIMENSION CHEML(201)
    COMMON /VBRCOM/ I,C02,WATVA,CDEXT,COEXB
    COMMON /ITRCOM/ ITER
    COMMON /POPCOM/ VIBPOP(201,25)
    COMMON /KCEM/KCHEM
    COMMON /INOUT/NR,NP,NW
    EQUIVALENCE (TDOWN2(1),TDOWN(1,9)),(TTUP2(1),TTUP(1,9))
    EQUIVALENCE (GNDSTE(1),VIBPOP(1,1))
    COMMON /TEQCOM/ NLTE
    COMMON /DEN(201,10),BNDTAU(201,25),BNDRAD(201,25),TEMP(201)
    1 ,BND,AM(25),DENTOT(201)
    DATA /FAC /1.0/
    RTFUN(NUS,NBS) =
    1 (XFER(VIBPOP(1,NUS),TTH(1,NBS),NZ,1,1,KB(NES)))

```

```

2  + XFER(VIBPOP(NZ,NUS),TTH(NZ,NBS),NALT,NZ,2,<3(NBS))) *EA(NBS)
3  +GDOWN(NBS)*SM1(KB(NBS),ZFAC*TTDOWN(NZ,NBS))
4  +GUP(NBS)*SLM1(KB(NBS),TTUP(NZ,NBS))
   AAA = 0.0
   IF (NLTE.EQ. 4) AAA = 2.0
   IF (KCHEM.EQ. 1) READ(NR,50) CHEML
50  FORMAT (6E12.4)
   IF (KCHEM.EQ. 1) KCHEM = 0
   DO 130 NZ = 1, NALT
     SUM = 0.0
     TMP = TEMP(NZ)
     DO 110 NL = 2, NLEVEL
       JL = (NL - 1)*25 + 1
       XYN = MOD(LSC(JL)/10,10)
       AA = EXP(-1.43879*WAVE(JL)/TMP)*XYN
       VIBPOP(NZ,NL) = AA
       SUM = SUM + AA
     CONTINUE
110  SUM = SUM + 1.0
       GNDSTE(NZ) = CONC(NZ)/SUM
       DO 120 NL = 2, NLEVEL
         VIBPOP(NZ,NL) = CONC(NZ)*VIBPOP(NZ,NL)/SUM
       CONTINUE
120  CONTINUE
130  CONTINUE
       DO 135 NL = 2, NLEVEL
         JL = (NL - 1)*25 + 1
         IF (LCC(JL).EQ. 1) VVWAVE = 2331.- WAVE(JL)
         IF (LCC(JL).EQ. 2) VVWAVE = 1556.4 - WAVE(JL)
         FAC = 2331.0
         IF (LCC(JL).EQ. 2) FAC = 1556.4
       CONTINUE
135  IF(NLTE.EQ.1) GO TO 170

```

```

DO 160 NZ = 1,NALT
TEMPNZ = TEMP(NZ)
TEMP13 = EXP(ALOG(TEMPNZ)/3.0)
IF (I .EQ. 3) GO TO 136
IF (I .NE. 2) GO TO 140
VTSIG(NZ) = 6.69E-10*EXP(-84.07/TEMP13)
VVRSIG(NZ) = 1.71E-6*EXP(-175.3/TEMP13)
1 + 6.07E-14*EXP(15.27/TEMP13)
VJSIG(NZ) = 1.0E-15 + 5.16E-11*EXP(-76.75/TEMP13)
VNVSIG(NZ) = VVRSIG(NZ)/EXP(1.43879/TEMP(NZ)*18.0)
VVJSIG(NZ) = VVDSIG(NZ)*VIBPOP(NZ,8)/VIBPOP(NZ,5)
GO TO 150
136 CONTINUE
FAC = 0.0
VVNSIG(NZ) = 4.0E-13
VTSIG(NZ) = 5.37E-10*EXP(-70.0/TEMP13)
VVRSIG(NZ) = VNVSIG(NZ)*EXP(-1.43879/TEMP(NZ)*1594.736)
GO TO 150
140 CONTINUE
VTSIG(NZ) = CDEXT(I)
VNVSIG(NZ) = CDEXB(I)
VVRSIG(NZ) = VNVSIG(NZ)*EXP(-1.43879/TEMP(NZ)*VVWAVE)
150 CONTINUE
TVSIG(NZ) = VTSIG(NZ)/GNDSTE(NZ)*VIBPOP(NZ,2)
VTSIG(NZ) = VTSIG(NZ)*DENTOT(NZ)
TVSIG(NZ) = TVSIG(NZ)*DENTOT(NZ)
TNV = TEMP(NZ)
IF (NLT. 5) GO TO 154
IF (N7 .GT. 41 .AND. NZ .LT. 51) TNV = TEMP(NZ)+FLOAT(NZ-41)
1 + 28.0
IF (N7 .GE. 51) TNV = 3000.0
154 CONTINUE

```

```

160 FACTOR = EXP(-1.43879*FAC/T*INV)
    VVNSIG(NZ) = VVNSIG(NZ)*DENTOT(NZ)*FACTOR/(1.0 + FACTOR)
    VVRSIG(NZ) = VVRSIG(NZ)*DENTOT(NZ)/(1.0 + FACTOR)
    CONTINUE
    DO 166 NZ = 1, NALT
        SUM = 0.0
        TMP = 180.0
        DO 162 NL = 2, NLEVEL
            JL = (NL - 1)*25 + 1
            XYN = MOD(LSC(JL)/10,10)
            AA = EXP(-1.43879*WAVE(JL)/TMP)*XYN
            VIBPOP(NZ,NL) = AA
            SUM = SUM + AA
        162 CONTINUE
        SUM = SUM + 1.0
        GNDSIG(NZ) = CONC(NZ)/SUM
        DO 164 NL = 2, NLEVEL
            VIBPOP(NZ,NL) = CONC(NZ)*VIBPOP(NZ,NL)/SUM
        164 CONTINUE
        166 CONTINUE
        170 CONTINUE
        DO 175 IX = 1, NALT
            CONTINUE
        175 DO 180 NB = 1, NBAND
            NBX = (NB - 1)*25 + 1
            NBC = LBC(NBX)
            NI = MOD(NBC/100,100)
            NF = MOD(NBC,100)
            JI = (NI - 1)*25 + 1
            JF = (NF - 1)*25 + 1
            KL(NB) = MOD(LBU(NBX)/10,10)
            KB(NB) = MOD(LBU(NBX),10)

```



```

1290 THAVE = WAVE(JI) - WAVE(JF)
1300 BNOLAM(NB) = 1.0E+4/THAVE
1310 IF (TFLUX(NB) .EQ. 0.0) TFLUX(NB) =
1320 1 5.997E+6*THAVE**4/(EXP(1.43879*THAVE/TEMP(1)) - 1.0)
1330 XYM = MOD(LSC(JF)/10,10)
1340 XYM4 = MOD(LSC(JI)/10,10)
1350 EA(NB) = STR(NBX)*2.804/BNOLAM(NB)**2*XYM
1360 1 *EXP(1.43879*WAVE(JF)/300.0)/XYMM
1370 POWER(NB) = 1.58065E-20/BNOLAM(NB)
1380 GFAC(NB) = 3.72E-24*STR(NBX)*BNOLAM(NB)**2
1390 1 *EXP(1.43879*WAVE(JF)/296.0)
1400 GUP(NB) = GFAC(NB)*TFLUX(NB)*12.4864
1410 IF (NLTE .LT. 3) GUP(NB) = 0.0
1420 GDOWN(NB) = GFAC(NB)*SFLUX(NB)
1430 IF (NLTE .LT. 4) GDOWN(NB) = 0.0
1440 KBN = <8(NB)
1450 KLV = <L(NB)
1460 BNOL = BNOLAM(NB)
1470 FAC = POWER(NB)*EA(NB)
1480 SNB = STR(NBX)*EXP(1.43879*WAVE(JF)/296.0)
1490 DO 180 NZ = 1, NALT
1500 BNJTAU(NZ,NB) = TAUMAX(KLN,KBN,RM,BV,TEMP(NZ),BNOL,SNB,
1510 1 VIRPOP(NZ,NF))
1520 IF (NLTE .GT. 1) GO TO 180
1530 BNJPAO(NZ,NB) = VIRPOP(NZ,NI)*FAC
1540 CONTINUE
1550 180 IF (NLTE .EQ. 1) GO TO 900
1560 ITMAX = 4
1570 IF (I .EQ. 2) ITMAX = 10
1580 ITER = 3
1590 181 ITER = ITER + 1
1600 NMIN = NALT - 1

```

```

1610 DO 190 NB = 1, NBAND
1620   TTDOWN(NALT,NB) = 0.0
1630   TTUP(1,NB) = 0.0
1640   TTH(1,NB) = SIMP(BNDTAU(1,NB),1.0E+5,1)
1650 DO 182 NZ = 2, NMIN
1660   TTH(NZ,NB) = SIMP(BNDTAU(NZ - 1,NB),1.0E+5,2)
1670   CONTINUE
1680 DO 184 NZ = 2, NMIN
1690   NY = NALT - NZ + 1
1700   TTUP(NZ,NB) = TTUP(NZ - 1,NB) + TTH(NZ - 1,NB)
1710   TTDOWN(NY,NB) = TTDOWN(NY + 1,NB) + TTH(NY,NB)
1720   CONTINUE
1730   TTDOWN(1,NB) = TTDOWN(2,NB) + TTH(1,NB)
1740   TTUP(NALT,NB) = TTUP(NMIN,NB) + TTH(NMIN,NB)
1750   IF (NLT - GT. 3) GO TO 190
1760 DO 186 NZ = 1, NALT
1770   TTDOWN(NZ,NB) = 0.0
1780   CONTINUE
1790   IF (NLT - GT. 2) GO TO 190
1800 DO 188 NZ = 1, NALT
1810   TTUP(NZ,NB) = 0.0
1820   CONTINUE
1830   CONTINUE
1840   CONTINUE
1850   GO TO (210,220,230,240,250,260,260), I
1860   CONTINUE
1870 DO 215 NZ = 1, NALT
1880   VIBPOP(NZ,3) = GNDSTE(NZ)*(GUP(2)*SLM1(KB(2),TTUP(NZ,2))
1890     + GDOWN(2)*SM1(KB(2),TTDOWN(NZ,2)))/(EA(2) + EA(4))
1900   VIBPOP(NZ,2) = (EA(4)*VIBPOP(NZ,3) + GNDSTE(NZ)
1910     *(GUP(1)*SLM1(KB(1),TTUP(NZ,1))
1920     + GDOWN(1)*SM1(KB(1),TTDOWN(NZ,1)))

```

```

1930
1940
1950
1960
1970
1980
1990
2000
2010
2020
2030
2040
2050
2060
2070
2080
2090
2100
2110
2120
2130
2140
2150
2160
2170
2180
2190
2200
2210
2220
2230
2240

3 + TVSIG(NZ) + 0.75*VVNSIG(NZ)))
4 /(EA(1) + VTSIG(NZ) + 0.75*VVRSIG(NZ))
VIBPOP(NZ,4) = GNDSTE(NZ)*0.25*VVNSIG(NZ)
1 + GUP(3)*SLM1(KB(3),TTUP(NZ,3))
2 + GDOWN(3)*SM1(KB(3),TTDOWN(NZ,3)))
3 /(EA(3) + 0.25*VVRSIG(NZ))
215 CONTINUE
GO TO 350
220 CONTINUE
NZ = 0
221 NZ = NZ + 1
VIBPOP(NZ,8) = GNDSTE(NZ)*VVNSIG(NZ) + RTFUN(8,9))
2 /(VVRSIG(NZ) + EA(9) + VVDSIG(NZ))
TVS = TVSIG(NZ)
VTS = VTSIG(NZ)
POP3 = VIBPOP(NZ,3)
POP4 = VIBPOP(NZ,4)
POP7 = VIBPOP(NZ,7)
POP2 = ((TVS + RTFUN(2,1))*GNDSTE(NZ)
2 + POP3*(EA(2) + VTS) + POP4*(EA(3) + VTS)
3 + POP7*(EA(7) + VTS))/(VTS + EA(1) + TVS)
VIBPOP(NZ,2) = POP2
POP8 = VIBPOP(NZ,8)
POP7 = ((TVS*0.25 + GUP(7)*SLM1(KB(7),TTUP(NZ,7))
1 + GDOWN(7)*SM1(KB(7),TTDOWN(NZ,7)))*POP2
2 + EA(8)*POP8)/(EA(7) + VTS)
VIBPOP(NZ,7) = POP7
POP5 = VIBPOP(NZ,5)
POP6 = VIBPOP(NZ,6)
POP3 = (POP2*(0.25*TVS + GUP(2)*SLM1(KB(2),TTUP(NZ,2))
1 + GDOWN(2)*SM1(KB(2),TTDOWN(NZ,2))) + POP5*(EA(4) + VTS))
2 /(EA(2) + VTS + TVS)

```

```

2250      VIBPOP(NZ,3) = POP3
2260      POP4 = (POP2*(0.5*TVS + GUP(3)*SLM1(KB(3),TTJD(NZ,3))
2270      + GDOWN(3)*SM1(KB(3),TTDOWN(NZ,3))) + POP5*EA(5)
2280      + POP6*(EA(6) + VTS))/(EA(3) + VTS + TVS)
2290      VIBPOP(NZ,4) = POP4
2300      POP5 = (POP3*(TVS + GUP(4)*SLM1(KB(4),TTUP(NZ,4))
2310      + GDOWN(4)*SM1(KB(4),TTDOWN(NZ,4)))
2320      + POP4*(GUP(5)*SLM1(KB(5),TTUP(NZ,5))
2330      + GDOWN(5)*SM1(KB(5),TTDOWN(NZ,5))) + POP8*VVDSIG(NZ))
2340      /(EA(4) + EA(5) + VTS + VVUSIG(NZ))
2350      VIBPOP(NZ,5) = POP5
2360      POP6 = (POP4*(0.5*TVS + GUP(6)*SLM1(KB(6),TTJD(NZ,6))
2370      + GDOWN(6)*SM1(KB(6),TTDOWN(NZ,6)))/(EA(6) + VTS)
2380      + VIBPOP(NZ,6) = POP6
2390      GNDSTF(NZ) = CONC(NZ) - (POP8 + POP6 + POP5 + POP7 + POP4
2400      + POP3 + POP2)
2410      IF (GNDSTE(NZ) .LE. 0.0) GNDSTF(NZ) = 0.05*CONC(NZ)
2420      225 IF (NZ.LT.NALT) GO TO 221
2430      GO TO 350
2440      230 CONTINUE
2450      DO 235 NZ = 1, NALT
2460      VIBPOP(NZ,2) = ((TVSIG(NZ) + VVRSIG(NZ)
2470      + RTFUN(2,1))*GNDSTE(NZ) + VIBPOP(NZ,3)*EA(5))
2480      /(VTSIG(NZ) + EA(1) + VVNSIG(NZ))
2490      VIBPOP(NZ,3) = ((TVSIG(NZ) + VVRSIG(NZ)
2500      + RTFUN(3,5))*VIBPOP(NZ,2) +
2510      RTFUN(3,2)*GNDSTE(NZ) + VIBPOP(NZ,6)*EA(11))
2520      /(EA(2) + EA(5) + VTSIG(NZ) + VVNSIG(NZ))
2530      VIBPOP(NZ,4) = (RTFUN(4,3)*GNDSTE(NZ)
2540      + RTFUN(4,6)*GNDSTE(NZ))/(EA(3) + EA(6))
2550      VIBPOP(NZ,5) = (RTFUN(5,4)*GNDSTE(NZ)
2560      + RTFUN(5,7)*VIBPOP(NZ,2))/(EA(4) + EA(7))

```

```

2570      VIBPOP(NZ,6) = (RTFUN(6,8)*VIBPOP(NZ,8)
2580      1 + RTFUN(6,12)*GNDSTE(NZ))/(EA(8) + EA(11))
2590      2 + EA(12))
2600      VIBPOP(NZ,7) = (RTFUN(7,9)*VIBPOP(NZ,2)
2610      1 + RTFUN(7,13)*GNDSTE(NZ))/(EA(9) + EA(13))
2620      VIBPOP(NZ,8) = (RTFUN(8,10)*VIBPOP(NZ,2)
2630      1 + RTFUN(8,14)*GNDSTE(NZ))/(EA(10) + EA(14))
2640      235 CONTINUE
2650      GO TO 350
2660      240 CONTINUE
2670      DO 245 NZ = 1, NALT
2680      VIBPOP(NZ,2) = ((TVSIG(NZ) + VVNSIG(NZ)
2690      1 + GUP(1)*SLM1(KB(1),TTUP(NZ,1))
2700      2 + XFER(VIBPOP(1,2),TTH(1,1),NZ,1,1,KB(1)))
2710      3 + XFER(VIBPOP(NZ,2),TTH(NZ,1),NALT,NZ,2,KB(1)))*EA(1)
2720      4 + GDOWN(1)*SM1(KB(1),TTDOWN(NZ,1))*GNDSTE(NZ)
2730      5 + (EA(3) + VTSIG(NZ))*VIBPOP(NZ,3) + AAA*CHEML(NZ))
2740      5 / (EA(1) + VTSIG(NZ) + VVRSIG(NZ) + TVSIG(NZ))
2750      VIBPOP(NZ,3) = ((TVSIG(NZ)
2760      1 + GUP(3)*SLM1(KB(3),TTUP(NZ,3))
2770      2 + GUP(2)*SLM1(KB(2),TTUP(NZ,2))
2780      3 + GDOWN(2)*SLM1(KB(2),TTDOWN(NZ,2))
2790      4 + GDOWN(3)*SLM1(KB(3),TTDOWN(NZ,3))*VIBPOP(NZ,2)
2800      5 + AAA*CHEML(NZ))/(EA(2) + EA(3) + VTSIG(NZ))
2810      GNDSTE(NZ) = CONC(NZ) - VIBPOP(NZ,2) - VIBPOP(NZ,3)
2820      245 CONTINUE
2830      GO TO 350
2840      250 CONTINUE
2850      DO 255 NZ = 1, NALT
2860      VIBPOP(NZ,6) = GNDSTE(NZ)*(VVNSIG(NZ)
2870      1 + GDOWN(3)*SM1(KB(3),TTDOWN(NZ,3))
2880      2 + GUP(3)*SLM1(KB(3),TTUP(NZ,3)))

```

```

2890 3 / (VVRSIG(NZ)*1.5 + EA(3))
2900 VI3POP(NZ,5) = (VI3POP(NZ,6)*VVRSIG(NZ)*0.5
2910 1 + TVSIG(NZ)*VI3POP(NZ,4)) / (VSIG(NZ) + 5.0*EA(1))
2920 VI3POP(NZ,4) = (VI3POP(NZ,5) * (VSIG(NZ) + 5.3*EA(1))
2930 1 + TVSIG(NZ)*VI3POP(NZ,3))
2940 2 / (VSIG(NZ) + VSIG(NZ) + 4.0*EA(1))
2950 VI3POP(NZ,3) = (VI3POP(NZ,4) * (VSIG(NZ) + 4.0*EA(1))
2960 1 + TVSIG(NZ)*VI3POP(NZ,2)) / (VSIG(NZ) + VSIG(NZ) + 3.0*EA(1))
2970 VI3POP(NZ,7) = (VNSIG(NZ)*VI3POP(NZ,3)
2980 1 + GNDSTE(NZ)*(GUP(2)*SLM1(KB(2),TTUP(NZ,2))
2990 2 + GDOWN(2)*SM1(KB(2),TTDOWN(NZ,2))) / EA(2)
3000 VI3POP(NZ,2) = (GNDSTE(NZ) * (TVSIG(NZ)
3010 1 + GUP(1)*SLM1(KB(1),TTUP(NZ,1))
3020 2 + GDOWN(1)*SM1(KB(1),TTDOWN(NZ,1)))
3030 3 + VI3POP(NZ,3) * (3.0*EA(1) + VSIG(NZ)))
3040 4 / (VSIG(NZ) + TVSIG(NZ) + EA(1))
3050 255 CONTINUE
3060 GO TO 350
3070 260 CONTINUE
3080 DO 265 NZ = 1, NALT
3090 VI3POP(NZ,2) = (TVSIG(NZ) + VNSIG(NZ)
3100 1 + GUP(1)*SLM1(KB(1),TTUP(NZ,1))
3110 2 + XFER(VI3POP(1,2),TTH(1,1),NZ,1,1,KB(1))
3120 3 + XFER(VI3POP(NZ,2),TTH(NZ,1),NALT,NZ,2,KB(1)) * EA(1)
3130 4 + GDOWN(1)*SM1(KB(1),TTDOWN(NZ,1)) * GNDSTE(NZ)
3140 5 / (VSIG(NZ) + EA(1) + VVRSIG(NZ))
3150 265 CONTINUE
3160 GO TO 350
3170 350 CONTINUE
3180 DO 360 NB = 1, NBAND
3190 FAC = POWER(NB)*EA(NB)
3200 NBX = (NB - 1)*25 + 1

```

```

3210 NPC = LBC(NBX)
3220 NI = MOD(NBC/100,100)
3230 NF = MOD(NBC,100)
3240 KLN = KL(NB)
3250 KRN = KB(NB)
3260 BNDL = BNDLAK(NB)
3270 JF = (NF - 1)*25 + 1
3280 SNR = STR(NBX)*EXP(1.43879*WAVE(JF)/300.))
3290 DO 350 NZ = 1, NALT
3300 BNDLAN(NZ,NB) = VIBPOP(NZ,NI)*FAC
3310 BNDTAU(NZ,NB) = TAUMAX(KLN,KRN,PM,BV,TEMP(NZ),BNDL,SNB,
3320 1 VIBPOP(NZ,NF))
3330 360 CONTINUE
3340 DO 350 TX = 1, NALT
3350 CONTINUE
3360 400 CONTINUE
3370 IF (ITER .LT. ITMAX) GO TO 181
3380 CONTINUE
3390 IF (NLTE .LE. 2) GO TO 920
3400 DO 310 NZ = 1, NALT
3410 WRITE (NP,9) (VIBPOP(NZ,NL), NL = 1, NLEVEL)
3420 CONTINUE
3430 920 CONTINUE
3440 RETURN
3450 8 FORMAT (1P8E10.4)
3460 15 FORMAT (1X)
3470 16 FORMAT (3X,1P10E12.4)
3480 26 FORMAT (6X,7I8)
3490 36 FORMAT (14I)
3500 END

```


Function XFER

Purpose:

Function XFER is used to compute the excitation of a vibrational level caused by molecules radiating in a given band.

Method:

Function XFER computes the contribution to the source function from the radiation received in a given vibration-rotation band by a molecule at a given altitude. A single entry to Function XFER computes this number for radiation received from molecules located either below or above this altitude. Equation (2-60) is summed over each altitude interval involved.

Program Flow:

Function XFER assumes that the values in RAD(1) and TTH(1) are the values corresponding to the lowest altitude over which the integration is to be performed. Thus when called from Subroutine BANRAD to determine the effect of molecules above a given altitude with index NZ, the calling argument list has the form (VIBPOP(NZ, 2), TTH(NZ, 1), NALT, NZ, 2, KB(1)) for a band transition between vibrational levels 1 and 2 and band number 1.

Upon entry to Function XFER, the number of altitude intervals is found from the difference of NTOP and NBOT, and stored in NINT. If NTOP = NBOT, the value 0.0 is returned by Function XFER.

Otherwise, K is tested and control transferred to the appropriate part of the function.

When K is one, XFER computes the radiative contribution to excitation from layers below the altitude level for which the computation is made.

When K is two, the contribution from layers above is computed.

The computation from a single level is found in each passage through the loop ending with statement 120 (if K is one) or statement 220 (if K is two). Before entry to either loop, RA is set to one, TB to zero, and EA3 to zero. RFAC, the ratio of ground state to upper state vibrational populations is computed and SUM is set to one-half. Within the appropriate loop, TB is incremented by the optical thickness obtained from array TTH. $1/2 N_{12}(\tau)$ for the band is obtained from function SLM1 and the value stored in EB2. The band function $1/2 L_3(\tau)$ is computed from the value of $L_0(\tau)$ obtained by a call to function SL3 and $1/2 N_{12}(\tau)$ through use of the recurrence relation

$$\frac{1}{2} L_3(\tau) = \frac{1}{4} [L_0(\tau) + \tau N_{12}(\tau)]$$

Equation (2-60) is then applied and the result added to the value in SUM.

Mnemonic Variables:

EA3	Temporary storage for value of the band function L_3 for the nearer of two adjacent integration points
EB2	Temporary storage for value of the band function $1/2 N_{12}$ for the farther away of two adjacent integration points
EB3	Temporary storage for value of the band function L_3 for the farther away of two adjacent integration points
K	integer parameter used to choose appropriate section of this function
KB	integer parameter used to choose appropriate sections of functions SLM1 and SL3
NBOT NTOP	indices in altitude array of top and bottom altitudes in layer of interest
NF	index used to select values from array VIBPOP
NINT	(NTOP -- NBOT), number of intervals
NPL	(NINT + 1)
NY	index for altitude level
NZ	index for altitude level
RA	relative vibrational population of nearer altitude point
RAD	real array containing vibrational population of an upper state
RB	relative vibrational population of farther altitude point
RFAC	ratio of ground state population to upper vibrational level population
SUM	immediate result of integration

TB	optical distance from level for which calculation is being made to farther of two levels
TM	increment of optical thickness between two adjacent levels
TTH	real array storing incremental optical thicknesses
VIBPOP	real array storing vibrational populations of ground and excited levels of a molecule

Non-Library

Externals: SLM1, SL3

Called by: BANRAD

```

100      FUNCTION XFER (RAD,TTH,NTOP,NBOT,K,KB)
110      COMMON /POPCOM/ VIBPOP(201,25)
120      DIMENSION RAD(201),TTH(201),HOLD(201)
130      NINT = NTOP - NBOT
140      NN = NINT/2
150      KK = MOD(NINT,2)
160      NPL = NINT + 1
170      IF (NINT.GT. 0) GO TO 100
180      XFER = 0.0
190      RETURN
200      CONTINUE
210      RA = 1.0
220      TA = 0.0
230      TB = 0.0
240      EA3 = 0.0
250      IF (K.GT. 1) GO TO 200
260      NF = NFOP
270      RFAC = VIBPOP(NF,1)/RAD(NF)
280      SUM = 0.5*RA
290      DO 120 NZ = 1, NINT
300      NY = NINT - NZ + 1
310      TM = TTH(NY)
320      TB = TB + TM
330      EB2 = SLM1(KB,TB)
340      EB3 = (SL3(KB,TB) + 2.0*TB*EB2)/4.0
350      NF = NF - 1
360      RB = RFAC*RAD(NY)/VIBPOP(NF,1)
370      SUM = SUM + (RB - RA)*(EB3 - EA3)/TM
380      RA = RB
390      EA3 = EB3
400      CONTINUE
410      XFER = ABS(SUM - RB*EB2)/RFAC

```

```

200 RETURN
CONTINUE
NF = N30T
RFAC = VIBPOP(NF,1)/RAD(1)
SUM = 0.5*RA
DO 220 NZ = 2, NPL
  TM = TTH(NZ - 1)
  TB = TM + TM
  EB2 = SLM1(KB, TB)
  EB3 = (SL3(KB, TB) + 2.0*TB*EB2)/4.0
  NF = NF + 1
  RB = RFAC*RAD(NZ)/VIBPOP(NF,1)
  SUM = SUM + (RB - RA)*(EB3 - EA3)/TM
  RA = RB
EA3 = EB3
220 CONTINUE
XFER = ABS(SUM - RB*EB2)/RFAC
RETURN
END

```

Function SL3

Purpose:

This function yields the total absorption of radiation from a continuum source passing through a line absorbing medium. The result of this computation is used by function XFER to compute the band function $L_3^b(\tau)$.

Method:

SL3 computes the function $L^b(\tau)$ for parallel and perpendicular transitions in linear molecules. The algorithm uses a polynomial approximation to values of $L^b(\tau)$ computed for a reduced rotational temperature $hcB_v/kT = 0.002$. The values computed by SL3 are within five percent of the correct values for any reduced rotational temperature encountered in running the program.

Program Flow:

Upon entry, the absolute value of the argument TAU is defined as T. Some logic then is used to choose the appropriate polynomial curve fit to the function which is computed and return is executed.

Inputs:

K, TAU

Output:

SLM1

Mnemonic Variables:

K	input parameter used to choose appropriate branch of the function, K equals 1 for parallel band, K equals 2 for perpendicular band.
SL3	computed value of $L^b(\tau)$.

T	absolute value of argument of TAU
TAU	input variable, optical depth k_t .
X	argument used to compute curve fit
Y	natural logarithm of T.

Non-Library

Externals:

None

Called by:

XFER

```

10  FUNCTION SL3 (K,TAU)
20  T = ABS (TAU)
30  IF (K .EQ. 2) GO TO 200
40  IF (T .GT. 4.0) GO TO 110
50  X = (T - 2.0)*0.5
60  SL3 = (((0.0004110*X - 0.0018496)*X + 0.0353378)*X
70  1 - 0.0246060)*X + 0.0792553)*X - 0.2301023)*X + 0.6569377)*T
80  RETURN
90
100 110 CONTINUE
110 IF (T .GT. 10.0) GO TO 120
120 X = (T - 7.0)/3.0
130 SL3 = (((0.0001916*X - 0.0007254)*X + 0.0323078)*X
140 1 - 0.0080348)*X + 0.0274865)*X - 0.0942082)*X + 0.3539295)*T
150 RETURN
160 120 CONTINUE
170 Y = ALOG(T)
180 IF (T .GT. 100.0) GO TO 130
190 X = 9.210340371975/Y - 3.0
200 SL3 = (((0.0000869*X - 0.0001530)*X - 0.0331490)*X
210 1 + 0.0013943)*X - 0.0063660)*X + 0.0837053)*X + 1.1415564)*Y
220 RETURN
230 130 CONTINUE
240 X = 9.210340371975/Y - 1.0
250 SL3 = (((0.007142 - 0.006222*X) + 0.005211)*X
260 1 - 0.004896)*X - 0.005477)*X + 0.007743)*X - 0.015900)*X
270 2 + 0.122528)*X + 0.940111)*Y
280 RETURN
290 200 CONTINUE
300 IF (T .GT. 4.0) GO TO 210
310 X = (T - 2.0)*0.5
320 SL3 = (((0.0002431*X - 0.0010991)*X + 0.0341830)*X
1 - 0.0160764)*X + 0.0581769)*X - 0.2013270)*X + 0.7188944)*T

```

```

210 RETURN
    CONTINUE
    IF (T.GT. 10.0) GO TO 220
    X = (T - 7.0)/3.0
    SL3 = (((0.0001163*X - 0.0004699)*X + 0.0015637)*X
1      - 0.0065345)*X + 0.0255562)*X - 0.1003592)*X + 0.4282944)*T
    RETURN
220 CONTINUE
    Y = ALG(T)
    X = 4.50517018598309/Y - 1.0
    SL3 = (((0.035431 - 0.035886*X)*X + 0.052211)*X
1      - 0.036895)*X - 0.046818)*X + 0.045072)*X + 0.009249)*X
2      - 0.00887)*X - 0.062059)*X + 0.163319)*X + 1.399769)*Y
    RETURN
    END
330
340
350
360
370
380
390
400
410
420
430
440
450
460
470

```

Function TAUMAX

Purpose: The purpose of this function is to compute the optical thickness of the strongest line in an infrared vibrational - rotational band.

Method: Function TAUMAX computes the optical thickness k_o at the center of the strongest line of a vibrational-rotational band of a linear molecule, assuming Doppler line shape.

Program Flow: The optical thickness at the center of a line with Doppler shape is

$$k_o = 5.3612 \times 10^{-18} \sqrt{\frac{M}{T}} N_{lc} \lambda_o S_{lu}^{\text{line}}$$

where M is the molecular mass (gm/mole), T is the absolute temperature (K), N_{lc} is the columnar number density (molecules/cm⁻²), λ_o is the line center wavelength (μm) and S_{lu}^{line} is the line strength in absorption (cm⁻¹ (atm-cm)⁻¹) at 300 K. Function TAUMAX computes the reduced rotational temperature hcB_v/kT and transmits this as an argument to Function SJMAX which computes the fraction of total band strength in the strongest line $S_{J_{\text{max}}} / S_{lu}^{\text{band}}$. TAUMAX then computes the optical thickness at the center of the strongest line, using $S_{J_{\text{max}}}$ in place of S_{lu}^{line} in the above expression.

Inputs: KL, KB, RM, BV, T, FLAM, S, DEN

Output: TAUMAX

Mnemonic Variables:

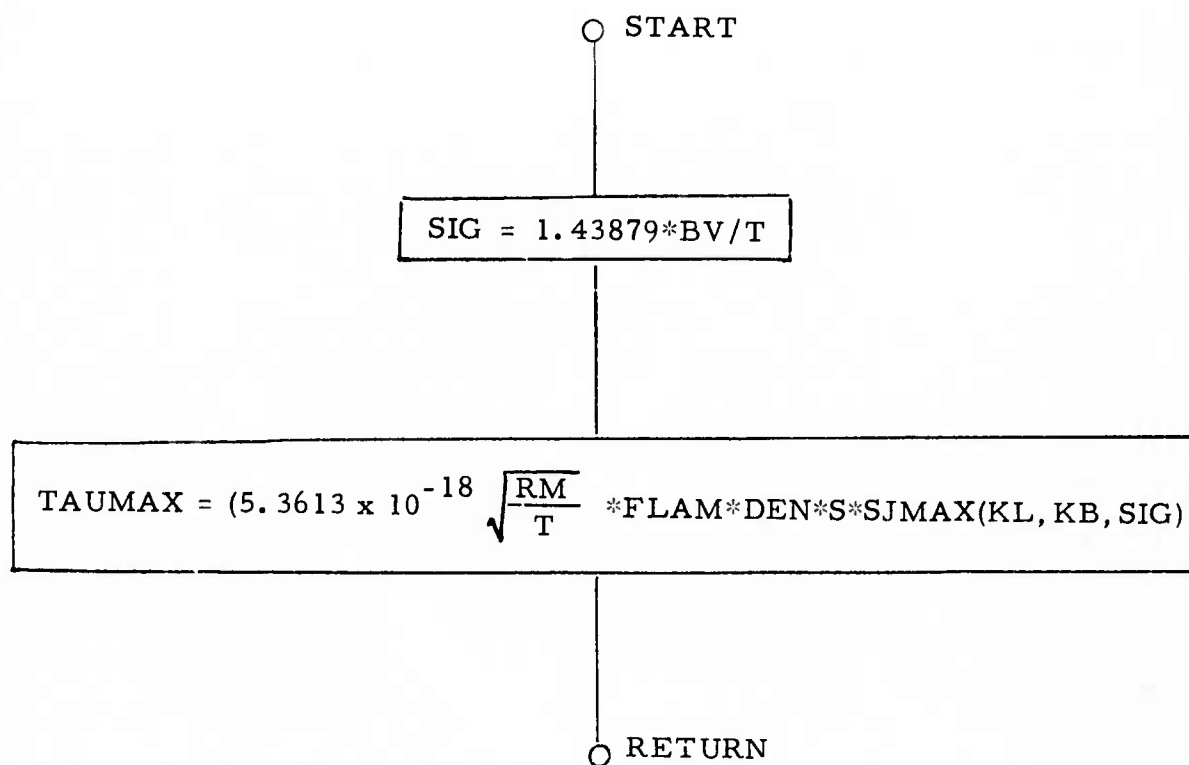
BV	rotational constant (cm^{-1})
DEN	columnar number density of molecule (cm^{-2})
FLAM	wavelength (μm)
KB	integer parameter
KL	integer parameter
RM	mass of molecule (gm/mole)
S	band strength ($\text{cm}^{-1}(\text{atm-cm})^{-1}$)
SIG	the quantity hcB_v/kT
T	temperature (K)
TAUMAX	value of optical thickness returned by function.

Non-Library

Externals: SJMAX

Called By: BANRAD

FLOW CHART: TAUMAX



```

FUNCTION TAUMAX (KL, KB, RM, BV, T, FLAM, S, DEN)
  SIG = 1.43879*BV/T
  TAJMAX = 5.3613E-18*SQRT(RM/T)*FLAM*DEN*S*SJMAX (KL, KB, SIG)
  RETURN
END

```

```

10
20
30
40
50

```


Function SJMAX

Purpose: The purpose of this function is to compute relative line strengths.

Method: Function SJMAX computes the relative strength of the strongest line in a parallel or perpendicular band of a linear molecule, assuming that all parallel bands are $1 \sum - 1 \sum$ transitions and all perpendicular bands are $1 \pi - 1 \sum$ transitions. The effect of neglecting the actual transition involved is negligible for the uses of Function SJMAX.

Program Flow: Function SJMAX computes the J values of the strongest line in the band, computes the strength from the appropriate Hönl-London formula, and divides this by the rotational partition function returned by Function QJPART.

Inputs: KL, KB, SIG

Output: SJMAX

Mnemonic Variables:

A	intermediate result in calculation
KB	parameter to choose type of transition (KB = $1 \sum - \sum$ transition) (KB = $2 \pi - \sum$ transition)
KL	parameter passed to QJPART

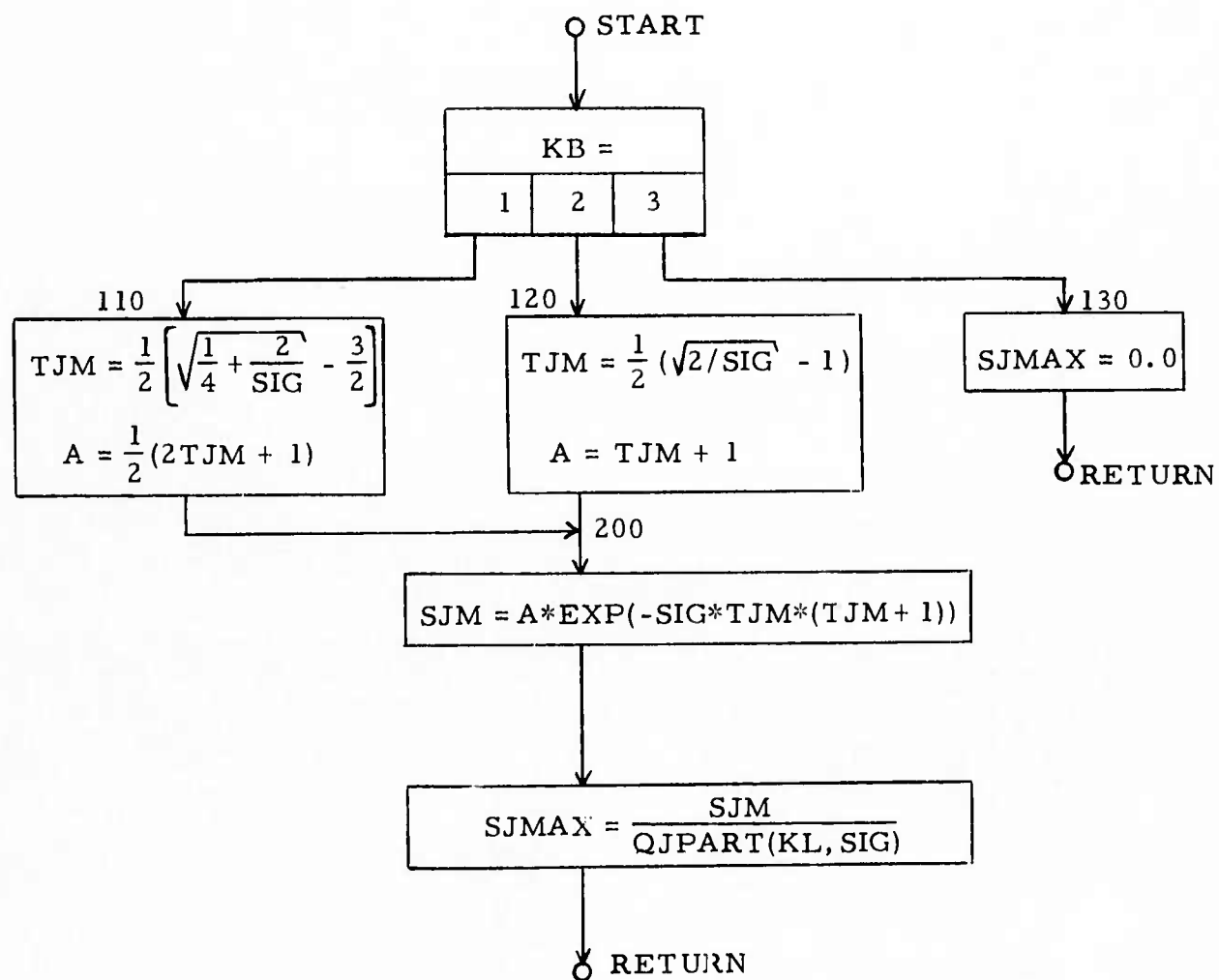
SIG the quantity $(hcB_v)/kT$
SJM strength of strongest line in band
SJMAX relative strength of strongest line in band
TJM effective rotational quantum number

Non-Library

Externals: QJPART

Called By: TAUMAX

FLOW CHART: SJMAX



C	FUNCTION SJMAX (KL,KB,SIG)	10
C	SJMAX COMPUTES THE RELATIVE STRENGTH OF THE STRONGEST LINE	20
C	IF KR = 1, SIGMA-SIGMA TRANSITION	30
	IF KR = 2, SIGMA-PI TRANSITION	40
	GO TO (110,120,130), KB	50
110	CONTINUE	60
	TJM = .5*(SQRT(0.25 + 2.0/SIG) - 1.5)	70
	A = 0.5*(TJM + TJM + 1.0)	80
	GO TO 200	90
120	CONTINUE	100
	TJM = .5*(SQRT(2.0/SIG) - 1.0)	110
	A = TJM + 1.0	120
	GO TO 200	130
130	CONTINUE	140
	SJMAX = 0.0	150
	RETURN	160
200	CONTINUE	170
	SJM = A*EXP(-SIG*TJM*(TJM + 1.0))	180
	SJMAX = SJM/QJPART(KL,SIG)	190
	RETURN	200
	END	210

Function QJPART

Purpose: The purpose of this function is to compute rotational partition functions for linear molecules. Refer to Subroutine BANRAD for definition of symbols.

Method: Function QJPART computes the rotational partition function of a single vibrational level of a rigid linear molecule, assuming that the energy E_J of a rotational state with quantum number J is

$$E_J = hcB_v J(J+1)$$

Provision is made for computing the rotational partition functions for vibrational levels in which rotational states with only even or odd J values are present.

Program

Flow:

If I all rotational levels are assumed populated.
If $K = 2$, only even rotational levels are assumed populated. If $K = 3$, only odd rotational level are assumed populated.

The computation uses polynomial approximates to the partition function

$$Q_J = \sum_J (2J+1) \exp(-E_J/kT)$$

with SIG as the parameter. The range of applicability is limited to values of SIG less than 0.2, and the largest value of SIG encountered for the molecules presently included is 0.015.

Inputs: K, SIG

Outputs: QJPART

Menemonic Variables:

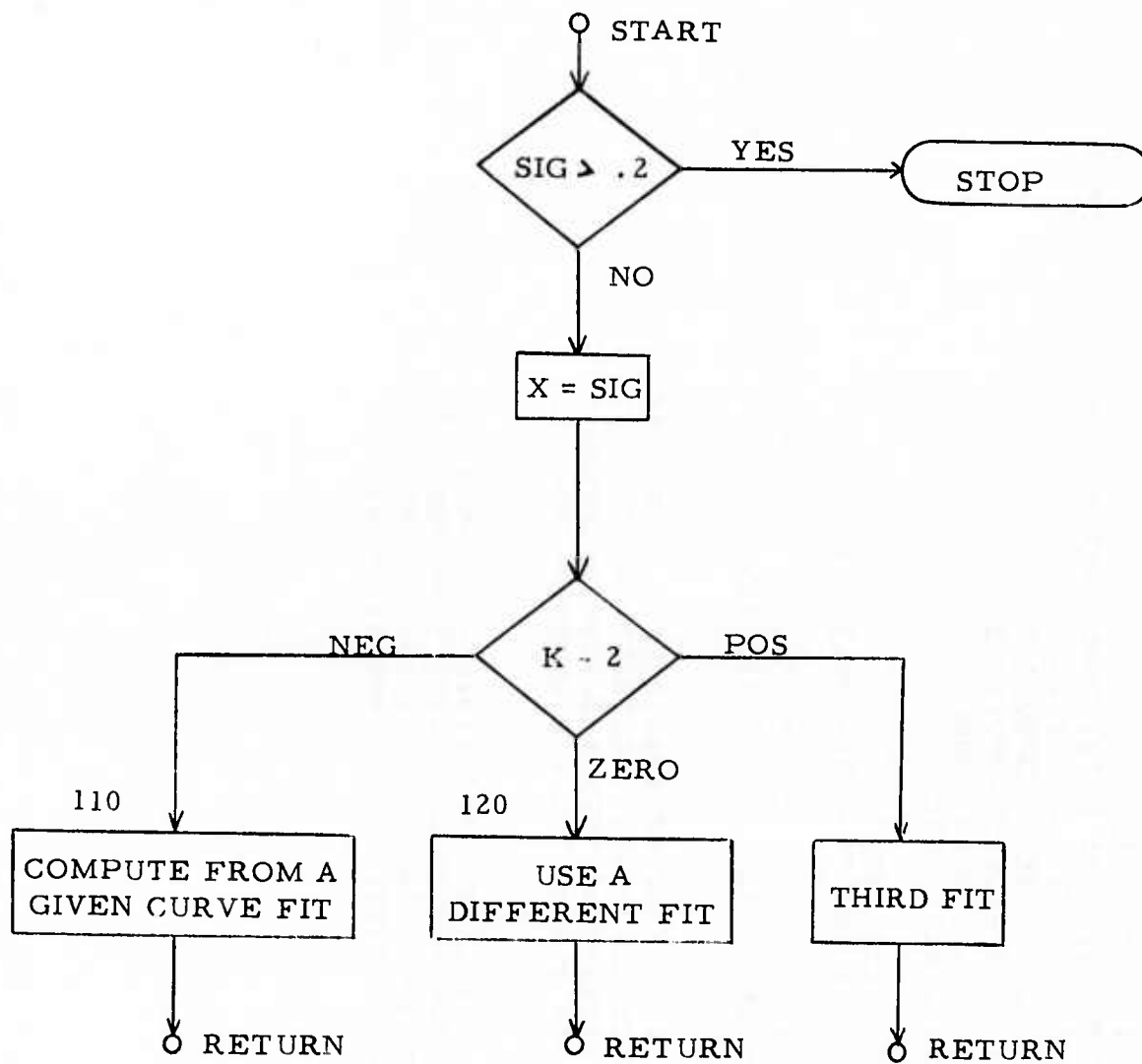
K	parameter used to choose appropriate fit
QJPART	value of rotational partition function
SIG	the quantity (hcB_v/kT)
X	the value of SIG, defined for convenience in the curve fit

Non-Library

Externals: None

Called By: SJMAX

FLOW CHART: QJPART




```

10
20
30
40
50
60
70
80
90
100
110
120
130
140
150
160
170
180
190
200
210
220
230
240
250
260
270

FUNCTION QJPART (K,SIG)
  QJPART COMPUTES THE ROTATIONAL PARTITION FUNCTION FOR A
  RIGID ROTATOR, SIG .LE. 0.2.
  K = 1, ALL LEVELS POPULATED
  K = 2, EVEN LEVELS POPULATED
  K = 3, ODD LEVELS POPULATED
  IF (SIG .GT. 0.2) STOP
  X = SIG
  IF (K - 2) 110,120,130
  COEFFICIENTS ARE FROM RUN DALTE-EV
  110 CONTINUE
  QJPART = (((0.00386500232857*SIG + 0.0125718935471)*X
    + 0.0666756164530)*X + 0.333333133379)*X + 1.0000000017)/SIG
  1 RETURN
  120 CONTINUE
  QJPART = ((((((62.5879214103*SIG - 29.5697177693)*SIG
    + 5.49692670096)*SIG - 0.502572235608)*SIG
    + 0.0297378193546)*SIG + 0.0328350909505)*SIG
    + 0.166670220770)*SIG + 0.4999999999456)/SIG
  130 CONTINUE
  QJPART = ((((((29.5703117876 - 62.5874596502*SIG)*SIG
    - 5.49579373669)*SIG + 0.505750942701)*SIG
    - 0.0170397551676)*SIG + 0.0338315889063)*SIG
    + 0.166663112387)*SIG + .5000000000544)/SIG
  RETURN
  END

```

Function SIMP

Purpose: The purpose of this function is to compute an integral using Simpson's rule.

Method: Function SIMP computes the integral of a function between any two of three equally spaced points. Simpson's rule integration is used.

Program

Flow: Upon entry, the value of K is tested to choose the appropriate branch of the function with the following results:

$$K < 2 \quad \text{SIMP} = (h/12) (8A(2) + 5A(1) - A(3))$$

$$K = 2 \quad \text{SIMP} = (h/12) (8A(2) + 5A(3) - A(1))$$

$$K > 2 \quad \text{SIMP} = (h/3) (4A(2) + A(1) + A(3))$$

Inputs: A, H, K

Output: SIMP

Mnemonic Variables:

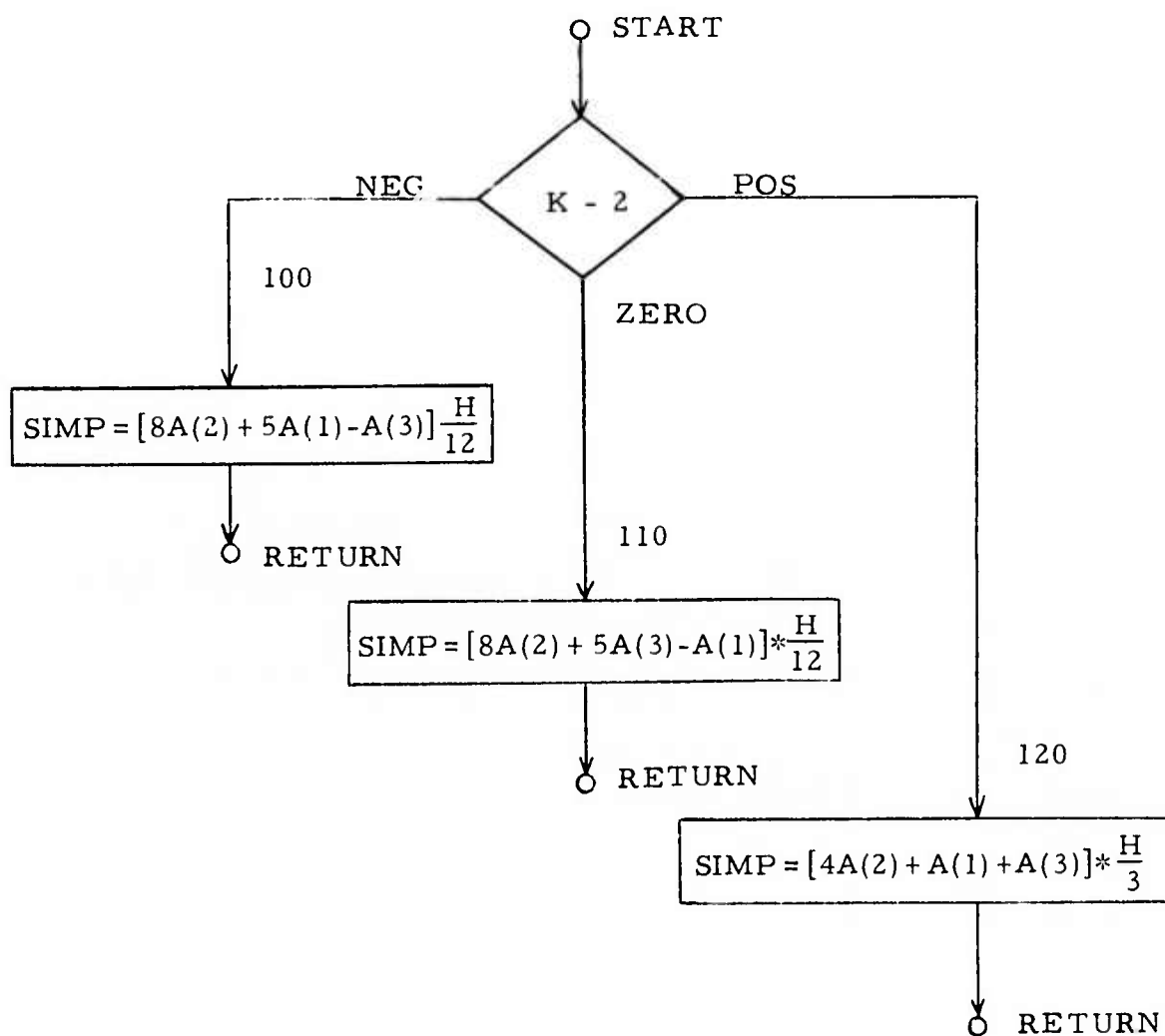
A	array of values to be integrated
H	integration step size
K	parameter to choose method desired

Non-Library

Externals: None

Called By: BANRAD, XFER

FLOW CHART: SIMP



```

FUNCTION SIMP (A,H,K)
  DIMENSION A(3)
  IF (K - 2) 100,110,120
100 CONTINUE
  SIMP = (8.0*A(2) + 5.0*A(1) - A(3))*H/12.0
  RETURN
110 CONTINUE
  SIMP = (8.0*A(2) + 5.0*A(3) - A(1))*H/12.0
  RETURN
120 CONTINUE
  SIMP = (4.0*A(2) + A(1) + A(3))*H/3.0
  RETURN
END

```

```

10
20
30
40
50
60
70
80
90
100
110
120
130

```

Function SM1

Purpose: This function yields a factor needed to compute the true rate of absorption at an optical depth, k_o , of radiation (from a spectrally constant source) in a resonant medium. Refer to Subroutine BANRAD for further explanation and definition of symbols used below.

Method: SM1 computes the function $M_1^b(k_o)$ for parallel and perpendicular transitions in linear molecules. The algorithm employs a polynomial approximation to values of $M_1^b(k_o)$ computed at a reduced rotational temperature $hcB_v/kT = 0.002$.

Program Flow: Upon entry the absolute value of the argument TAU is defined as T. Some logic then is used to choose the appropriate polynomial curve fit to the function which is computed and return is executed.

Inputs: K, TAU

Output: SM1

Mnemonic Variables:

K	input parameter used to choose appropriate branch of the function; K equals 1 for parallel band, K equals 2 for perpendicular band
SM1	rate of absorption at optical thickness k_o , relative to zero optical thickness
T	absolute value of argument TAU
TAU	input variable - optical depth k_o

Mnemonic Variables (Cont'd)

X	argument used to compute curve fit
Y	natural logarithm of T

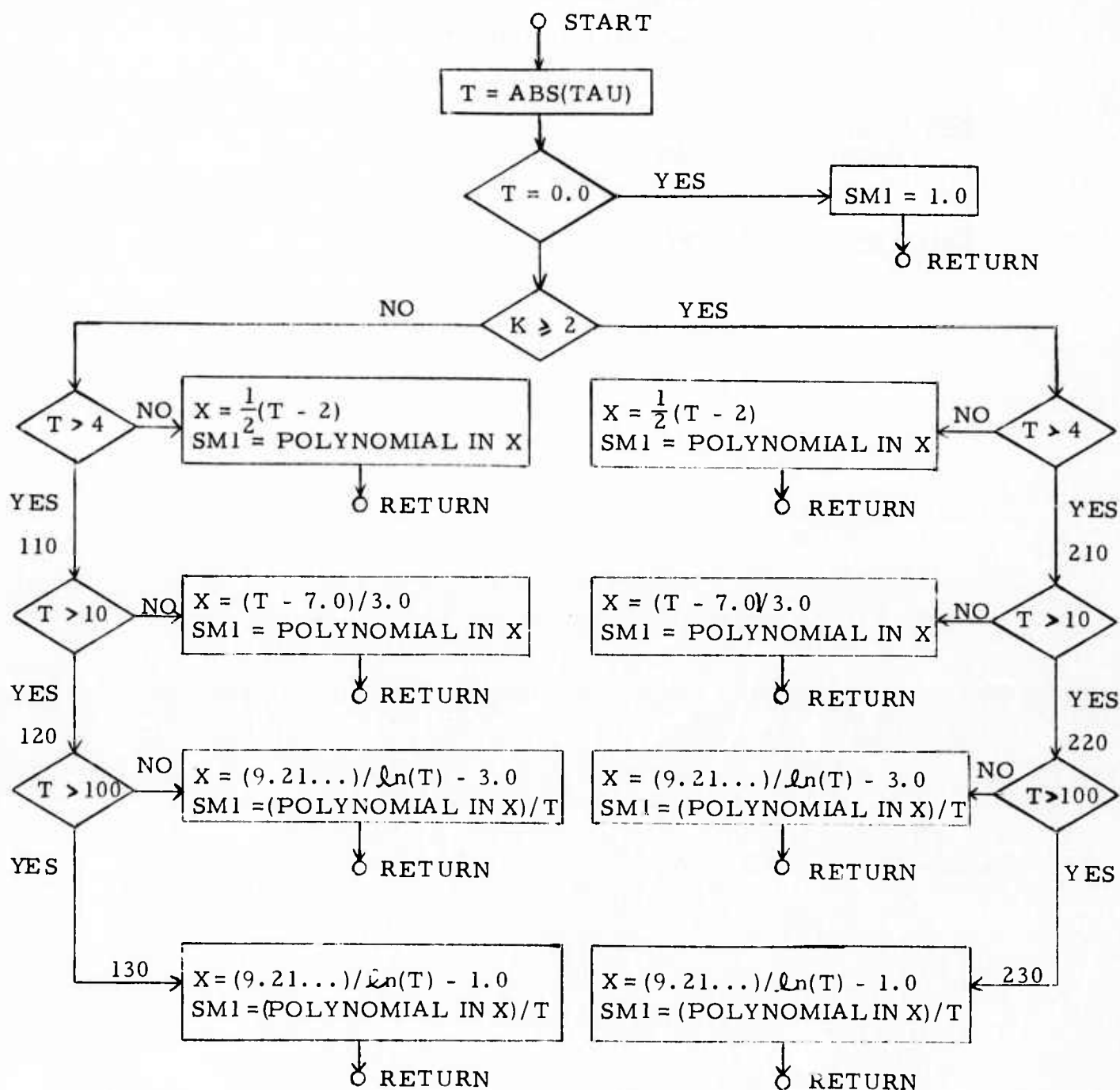
Non-Library

Externals: None

Called By: BANRAD

FLOW CHART:

SM1




```

10      FUNCTION SM1 (K,TAU)
20      T = ARS(TAU)
30      IF (T.EQ. 0.0) GO TO 300
40      IF (K.GE. 2) GO TO 200
50      IF (T.GT. 4.0) GO TO 110
60      X = (T - 2.0)*0.5
70      SM1 = (((2.35490E-03*X - 8.90535E-03)*X + 2.56223E-02)*X
80      - 7.07877E-02)*X + 1.63735E-01)*X - 3.01749E-01)*X + 0.426845
90      RETURN
100
110     CONTINUE
111     IF (T.GT. 10.0) GO TO 120
120     X = (T - 7.0)/3.0
130     SM1 = (((5.92297E-04*X - 1.79043E-03)*X + 4.05109E-03)*X
140     - 1.04749E-02)*X + 2.59109E-02)*X - 6.01708E-02)*X + 0.134123
150     RETURN
160
170     CONTINUE
171     IF (T.GT. 100.0) GO TO 130
180     Y = ALOG(T)
190     X = 9.210340371976/Y - 3.0
200     SM1 = ((((-6.24516E-04*X - 6.79378E-04)*X + 2.98590E-03)*X
210     - 1.29190E-03)*X - 6.31784E-03)*X + 3.78904E-02)*X
220     + 8.50441E-01)/T
230     RETURN
240
250     CONTINUE
251     Y = ALOG(T)
260     X = 9.210340371976/Y - 1.0
270     SM1 = (((6.12038E-04*X - 2.93434E-04)*X - 4.36163E-04)*X
280     + 1.70037E-02)*X - 3.80088E-04)*X + 3.23441E-02)*X
290     + 8.17407E-01)/T
300     RETURN
310
320     CONTINUE
321     IF (T.GT. 4.0) GO TO 210

```

```

330 X = (T - 2.0)*0.5
340 SM1 = (((1.39071E-03 *X - 5.29904E-03)*X + 1.58249E-02)*X
350 1 - 4.7+039E-02)*X + 1.26175E-01)*X - 2.86333E-01)*X + 0.517573
360 RETURN
370 210 CONTINUE
380 IF (T .GT. 10.0) GO TO 220
390 X = (T - 7.0)/3.0
400 SM1 = (((3.76420E-04*X - 1.25384E-03)*X + 3.41168E-03)*X
410 1 - 1.5360E-02)*X + 3.07476E-02)*X - 8.14705E-02)*X + 0.1941308
420 RETURN
430 220 CONTINUE
440 IF (T .GT. 100.0) GO TO 230
450 Y = ALG(T)
460 X = 9.210340371976/Y - 3.0
470 SM1 = (((-7.53415E-03*X - 8.87124E-03)*X + 6.52199E-02)*X
480 1 + 1.304245)/T
490 RETURN
500 230 CONTINUE
510 Y = ALG(T)
520 X = 9.210340371976/Y - 1.0
530 SM1 = (((1.99067E-03 - 5.82519E-04)*X)*X + 1.99669E-03)*X
540 1 + 1.2 174E-03)*X + 4.76165E-02)*X + 1.19445)/T
550 RETURN
560 300 CONTINUE
570 SM1 = 1.0
580 RETURN
590 END

```

Function SLM1

Purpose: This function yields the factor used to obtain the actual absorption of radiation from an extended black body surface passing through a resonant medium. Refer to Subroutine BANRAD for further explanation and definition of symbols used below.

Method: SLM1 computes the function $\frac{1}{2\pi} N_1^b(k_t)$ for parallel and perpendicular transitions in linear molecules. The algorithm uses a polynomial approximation to values of $\frac{1}{2\pi} N_1^b(k_t)$ computed for a reduced rotational temperature $hcB_v/kT = 0.002$. The values computed by SLM1 are within five percent of the correct values for any reduced rotational temperature encountered in running the program.

Program

Flow: Upon entry the absolute value of the argument TAU is defined as T. Some logic then is used to choose the appropriate polynomial curve fit to the function which is computed and return is executed.

Inputs: K, TAU

Output: SLM1

Mnemonic Variables:

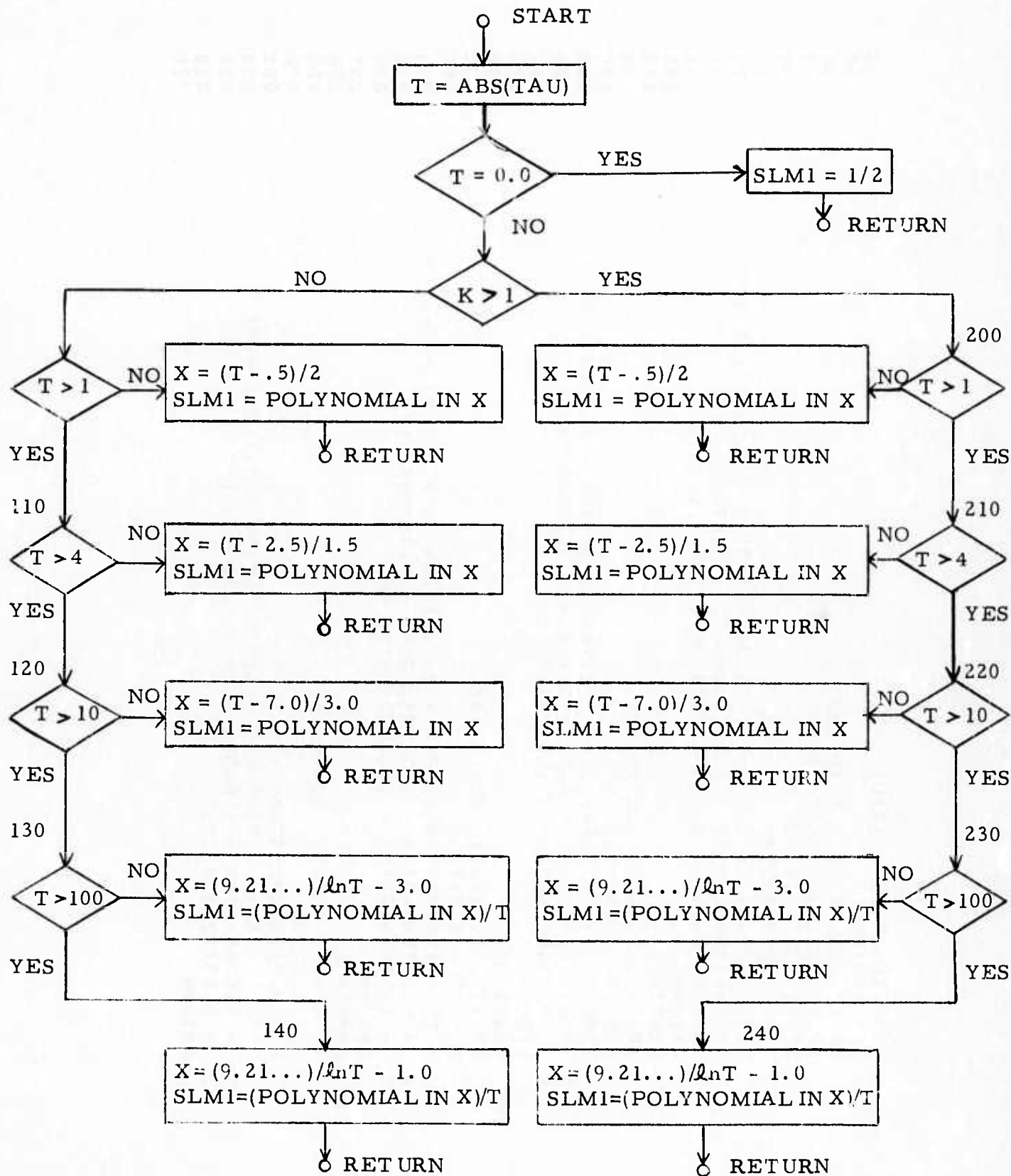
K	input parameter used to choose appropriate branch of the function, K equals 1 for parallel band, K equals 2 for perpendicular band
SLM1	computed value of $\frac{1}{2\pi} N_1^b(k_t)$
T	absolute value of argument TAU
TAU	input variable, optical depth k_t
X	argument used to compute curve fit
X	natural logarithm of T

Non-Library

Externals: None

Called By: BANRAD

FLOW CHART: SLM1



```

10  FUNCTION SLM1 (K,TAU)
20  T = ABS(TAU)
30  IF (T .EQ. 0.0) GO TO 300
40  IF (K .GT. 1) GO TO 200
50  IF (T .GT. 1.0) GO TO 110
60  T = 25.26760337*T
70  SLM1 = (((((5.54E-16*T - 1.3747E-13)*T + 3.11017E-11)*T
80  - 5.434609E-9)*T + 1.24762E-6)*T - 2.57626E-4)*T
90  - 7.08264246 + 0.01984964*ALOG(T))*T + 1.0)*0.5
100  RETURN
110  CONTINUE
111  IF (T .GT. 4.0) GO TO 120
120  X = (T - 2.5)/1.5
130  SLM1 = (((((3.00591E-3 - 1.41466E-3)*X - 3.88085E-3)*X
140  + 9.49736E-3)*X - 0.0239407)*X + 0.0523088)*X
150  - 0.1045984)*X + 0.1862743)*0.5
160  RETURN
170  CONTINUE
180  IF (T .GT. 10.0) GO TO 130
190  X = (T - 7.0)/3.0
200  SLM1 = (((((5.08470E-4 - 1.90181E-4)*X - 9.27594E-4)*X
210  + 2.24274E-3)*X - 5.54298E-3)*X + 0.01290804)*X
220  - 0.2939935)*X + 0.06552257)*0.5
230  RETURN
240  CONTINUE
250  IF (T .GT. 100.0) GO TO 140
260  Y = A-OG(T)
270  X = 9.210340371976/Y - 3.0
280  SLM1 = (((((7.836E-4)*X - 1.5181E-3)*X + 9.0128E-4)*X
290  - 6.498E-4)*X - 1.0632E-3)*X + 0.0149364)*X
300  + 0.4378273)*0.5/T
310  RETURN
320

```

```

140 CONTINUE
Y = ALOG(T)
X = 9.210340371976/Y - 1.0
SLM1 = (((5.0746E-3 - 4.681E-4*X)*X - 1.5848E-3)*X
1 + 0.0147526)*X + 0.4079074)*0.5/T
RETURN
200 CONTINUE
IF (T.GT. 1.0) GO TO 210
T = 26.0729185*T
SLM1 = (((((2.71E-16*T - 6.8372E-14)*T + 1.58314E-11)*T
1 - 3.33873E-9)*T + 7.01818E-7)*T - 1.61594E-4)*T
2 - 0.0356453 + 0.01494384*ALOG(T))*T + 1.0)*0.5
RETURN
210 CONTINUE
IF (T.GT. 4.0) GO TO 220
X = (T - 2.5)/1.5
SLM1 = (((((2.32E-3 - 1.1203E-3*X)*X - 3.0489E-3)*X
1 + 7.9345E-3)*X - 0.0213281)*X + 0.0521586)*X
2 - 0.1213660)*X + 0.2508902)*0.5
RETURN
220 CONTINUE
IF (T.GT. 10.0) GO TO 230
X = (T - 7.0)/3.0
SLM1 = (((((4.727E-4*X - 1.2459E-3)*X + 2.5253E-3)*X
1 - 6.7323E-3)*X + 0.0174769)*X - 0.0421443)*X
2 + 0.0958415)*0.5
RETURN
230 CONTINUE
IF (T.GT. 100.0) GO TO 240
Y = ALOG(T)
X = 9.210340371976/Y - 3.0
SLM1 = (((9.1E-5*X - 1.9096E-3)*X - 1.8059E-3)*X

```



```

1      + 0.0263129)*X + 0.6392594)*0.5/T
      RETURN
240    CONTINUE
      Y = ALG(T)
      X = 9.21034037976/Y - 1.0
      SL41 = (((6.444E-4)*X + 3.453E-4)*X - 5.099E-4)*X
      + 0.0216100)*X + 0.591052)*0.5/T
1      RETURN
300    CONTINUE
      SL41 = 0.5
      RETURN
      END

```

650
660
670
680
690
700
710
720
730
740
750
760

REFERENCES

- Abels, L.L. and Shaw, J. H., J. Mol. Spectrosc. 20, 11-28 (1966).
- Ackerman, M., Aeronomica Acta A, No. 62, Brussels (1970).
- Ackerman, M., Biaume, F. and Nicolet, M., Can. J. Chem. 47, 1834-1840 (1969).
- Anding, D., "Calculations of Atmospheric Spectral Radiance for Slant Paths from Several Altitudes", Report No. 8416-20-F(IV), Vol. IV, Willow Run Laboratories of the Institute of Science and Technology, The University of Michigan, Ann Arbor (1968).
- Anderson, J.G., J. Geophys. Res. 76, 4634-4652 (1971a).
- Anderson, J.G., J. Geophys. Res. 76, 7820-7824 (1971b).
- Arnold, J.O., Whiting, E.E., and Lyle, G.C., J. Quant. Radiat. Transfer 9, 775-798 (1969).
- Bainbridge, A.E., and Heidt, L.E., Tellus 18, 221-225 (1966).
- Barth, C.A., J. Geophys. Res. 69, 3301-3303 (1964).
- Barth, C.A., Planet. Space Sci. 14, 623 (1966a).
- Barth, C.A., Ann. Geophys. 22, 198-207 (1966b).
- Basco, N., Callear, A.B., and Norrish, R.G.W., Proc. Roy. Soc. A260, 459-474 (1961).
- Basco, N., Callear, A.B., and Norrish, R.G.W., Proc. Roy. Soc. A269, 180-187 (1962).
- Bates, D., and Hays, P., Planet. Space Sci. 15, 189-197 (1967).
- Bates, D.R., and Moiseiwitsch, B.L., J. Atmos. Terr. Phys. 8, 305-308 (1956).
- Bates, D.R., and Nicolet, M., Planet. Space Sci. 13, 905-909 (1965).
- Bates, D.R., and Witherspoon, A.E., Mon. Not. Roy. Astr. Soc. 112, 101-124 (1952).
- Bates, D.R., and Nicolet, M., J. Geophys. Res. 55, 301 (1950).
- Bauer, E., Kummier, R. and Bortner, M.H., App. Optics 10, 1861-1869 (1971).

- Bauer, S.H., and Tsang, S.C., Phys. Fluids 6, 182-189 (1963).
- Baulch, D.L., Drysdale, D.D., and Lloyd, A.C., "Critical Evaluation of Rate Data for Homogeneous, Gas-Phase Reactions of Interest in High-Temperature Systems", High Temperature Reaction Rate Data, No. 1, The University, Leeds, England, May (1968a).
- Baulch, D.L., Drysdale, D.D., and Lloyd, A.C., "Critical Evaluation of Rate Data for Homogeneous, Gas Phase Reactions of Interest in High-Temperature Systems", High Temperature Reaction Rate Data, No. 2, The University, Leeds, England, November (1968b).
- Baulch, D.L., Drysdale, D.D., Horne, D.G., and Lloyd, A.C., "Critical Evaluation of Rate Data for Homogeneous, Gas Phase Reactions of Interest in High-Temperature Systems", High Temperature Reaction Rate Data, No. 4, The University, Leeds, England, December (1968).
- Baulch, D.L., Drysdale, D.D., and Horne, D.G., "Critical Evaluation of Rate Data for Homogeneous, Gas Phase Reactions of Interest in High Temperature Systems, High Temperature Reaction Rate Data, No. 5, The University, Leeds, England, July (1970).
- Bérces, T., and Fürgeteg, S., Trans. Far. Soc. 66, 633-639 (1970a).
- Bérces, T., and Fürgeteg, S., Trans. Far. Soc. 66, 640-647 (1970b).
- Bérces, T., and Fürgeteg, S., Trans. Far. Soc. 66, 648-655 (1970c).
- Biondi, M.A., Can. J. Chem. 47, 1711-1719 (1969).
- Black, G., and Eckstrom, D. J., "Excitation and De-excitation of Vibration in N₂ by Oxygen Atoms", Final Report Contract DAHCO4-70-C-0036 ARPA Order No. 1482, SRI, Menlo Park, Calif., October (1971).
- Bowman, M.R., and Thomas, L., and Geisler, J.E., J. Atm. Terr. Phys. 32, 1661-1674 (1970).
- Breig, E.L., J. Chem. Phys. 51, 4539-4537 (1969).
- Brennan, W., and Niki, H., J. Chem. Phys. 42, 3725-3726 (1965).
- Bulirsch, R., and Stoer, J., Num. Math. 8, 1-13 (1966).
- Campbell, I.M., and Thrush, B.A., Trans. Far. Soc. 64, 1265-1274 (1968).

- Ceschino, F., and Kuntzmann, J., Numerical Solution of Initial Value Problems, Prentice-Hall, Englewood Cliffs. N. J. (1966).
- Chapman, S., and Cowling, T.G., The Mathematical Theory of Non-Uniform Gases, Cambridge University Press (1960).
- Clark, T.C., Garnett, S.H. and Kistiakowski, G.B., J. Chem. Phys. 52, 4692-4698 (1970).
- Clark, I.D., and Wayne, R.P., Proc. Roy. Soc. A316, 539-550 (1970).
- Clyne, M.A.A., and Thrush, B.A., Proc. Roy. Soc. A269, 404-418 (1962).
- Clyne, M.A.A., and Thrush, B.A., Proc. Roy. Soc. A275, 559 (1963).
- Colegrove, F.D., Johnson, F.S., and Hanson, W.B., J. Geophys. Res. 71, 2227-2236 (1966).
- Corbin, V.L., Dalgarno, A., Degges, T.C., House, F.B., Lilienfeld, P., Ohring, G., and Oppel, G.E., Atmospheric Radiance Models for Limb-Viewing Geometry in the Five- to Twenty-Five Micron Spectral Region, AFCRL-69-0552 (1969).
- Dalgarno, A., Planet. Space Sci. 10, 19-28 (1963).
- Dalgarno, A., Rev. Mod. Phys. 39, 858-861 (1967).
- Dalgarno, A., Phil. Trans. Roy. Soc. A264, 153-160 (1969).
- Dalgarno, A., Ann. Geophys. 26, 601-607 (1970).
- Davis, P.J., and Rabinowitz, P., Numerical Integration, Blaisdell, Waltham, Mass. (1967).
- Dalgarno, A., and McElroy, M.B., Planet. Space Sci. 14, 1321-1329 (1966).
- Dean, A.M., and Kistiakowsky, J. Chem. Phys. 54, 1718-1725 (1971).
- Degges, T.C., Applied Optics 10, 1856-1860 (1971).
- Degges, T.C., A High Altitude Radiance Model, AFCRL 72-0273 (1972).
- Detwiler, C.R., Garrett, D.L., Purcell, J.D., and Tousey, R., Ann. Geophys. 17, 263-272 (1961).
- Donahue, T.M., J. Geophys. Res. 71, 2237-2242 (1966).

- Donovan, R.J., and Hussain, D., Chem. Rev. 70, 489-510 (1970).
- Dunkin, D.B., Feasenfeld, F.C., Schmeltekopf, A.I., and Ferguson, E.E., J. Chem. Phys. 49, 1365-1371 (1968).
- Fehsenfeld, F.C., Schmeltekopf, A.L., Dunkin, D.B., and Ferguson, E.E., "Compilation of Reaction Rate Constants Measured in the ESSA Flowing Afterglow System to August 1969", ESSA Technical Report ERL 135-AL3, ESSA, Boulder, Colo., Sept. (1969).
- Fehsenfeld, F.C., Dunkin, D.B., and Ferguson, E.E., Planet. Space Sci. 18, 1267-1269 (1970).
- Feinberg, R.M., and Camac, M., Quant. Spectrosc. Radiat. Transfer 7, 581-590 (1967).
- Ferguson, E.E., Rev. Geophys. Space Phys. 9, 997-1008 (1971).
- Fisher, E.R., and Bauer, E., "The Quenching of $O(^1D)$ by N_2 ", presented at the DASA Symposium on Physics and Chemistry of the Upper Atmosphere, Philadelphia, Pa., 24-26 June (1970).
- Fite, W.L., Can. J. Chem. 47, 1797-1807 (1969).
- Foner, S.N., and Hudson, R.L., Chem. Phys. 36, 2681 (1962).
- Freedman, E., and Daiber, J.W., J. Chem. Phys. 34, 1271 (1961).
- Garnett, S.H., Kistiakowski, G.B., and O'Grady, B.V., J. Chem. Phys. 51, 84-91 (1969).
- Garvin, D., and Gevantman, L.H., "Chemical Kinetics Data Survey III. Selected Rate Constants for Chemical Reactions in Atmospheric Chemistry", NBS Report 10867, June 1972.
- Garvin, D., and Hampson, R.F., Editors, Chemical Kinetics Data Survey VII. Tables of Rate and Photochemical Data for Modelling of the Stratosphere (Revised). NBSIR 74-430, National Bureau of Standards, Washington, D.C., January (1974).
- Gear, C.W., Numerical Initial Value Problems in Ordinary Differential Equations, Prentice-Hall, Englewood Cliffs, N.J. (1971).
- Geissler, J.E., and Dickinson, R.E., J. Atmos. Terr. Phys. 30, 1505-1521 (1968).

- Gille, J.C., and Elingson, R.G., Appl. Op. 7, 471-474 (1968).
- Gilmore, F.R., Bauer, E., and McGowan, J.W., J. Quant. Spectrosc. Radiat. Transfer 9, 157-183 (1969).
- Goldan, P.D., Schmeltekopf, A.L., Fehsenfeld, F.C., Schiff, H.I., and Ferguson, E.E., J. Chem. Phys. 44, 4095-4103 (1966).
- Goody, R.M., Atmospheric Radiation, I, Theoretical Basis, Oxford University (1964).
- Hall, T.C., Jr., and Blacet, F.E., J. Chem. Phys. 20, 1745 (1952).
- Hampson, R.F., Brown, R.L., Garvin, D., Herron, J.T., Huie, R.E., McKinley, J.D., and Tsang, W., "Chemical Kinetics Data Survey I. Rate Data for Twelve Reactions of Interest for Stratospheric Chemistry", NBS Report 10692, January (1972a).
- Hampson, R.F., Braun, W., Garvin, D., Herron, J.T., Huie, R.E., Kurylo, M.J., Laufer, A.H., Okabe, H., and Tsang, W., "Chemical Kinetics Data Survey II. Photochemical and Rate Data for Fifteen Gas Phase Reactions of Interest for Stratospheric Chemistry", NBS Report 10828, April (1972b).
- Hays, P.B., and Olivero, J.J., Planet. Space Sci. 18, 1729-1733 (1970).
- Herron, J.T., Int. J. Chem. Kin. 1, 527-539 (1969).
- Herron, J.T., and Klein, F.S., J. Chem. Phys. 40, 2731 (1964).
- Herzberg, G., Molecular Spectra and Molecular Structure II. Infrared and Raman Spectra of Polyatomic Molecules, D. van Nostrand Co., Inc., New York (1945).
- Herzfeld, K.F., and Litovitz, T.A., Absorption and Dispersion of Ultrasonic Waves, Academic Press, New York (1959).
- Hesstvedt, E., Tellus 17, 341-349 (1965).
- Hesstvedt, E., Geophys. Norv. 27, No. 4, 1-35 (1968).
- Hoare, D.E., and Patel, M., Trans. Far. Soc. 65, 1325-1333 (1969).
- Houghton, J., Quart. J. Roy. Met. Soc. 95, 1-20 (1969).
- Hudson, R.D., Rev. Geophys. Space Sci. 9, 305-406 (1971).
- Hudson, R.D., and Carter, V.L., Can. J. Chem. 47, 1840-1844 (1969).

- Hudson, R.D., Carter, V.L., and Breig, E.L., J. Geophys. Res. 74, 4079-4086 (1969).
- Hunt, B.G., J. Atmos. Terr. Phys. 27, 133-144 (1965).
- Hunt, B.G., J. Geophys. Res. 71, 1385-1398 (1966).
- Hunten, D.M., and McElroy, M.B., Rev. Geophys. 4, 303-328 (1966).
- Hunten, D.M., and Strobel, D.F., "Production and Escape of Terrestrial Hydrogen", J. Atm. Sci. 31, 305-317 (1974).
- Hushfar, F., Rogers, J.W., and Stair, A.T., Jr., Appl. Optics 10, 1843-1847 (1971).
- Ivanov, V.V., "Approximate Solution to the Equation of Radiative Transfer in Line Frequencies", Soviet Astr. 16, 91-94 (1972).
- Ivanov, V.V., and Shcherbakov, V.T., Astrophysics 1, 10-16 (1965a).
- Ivanov, V.V., and Shcherbakov, V.T., Astrophysics 1, 17-22 (1965b).
- Ivanov, V.V., and Shcherbakov, V.T., Astrophysics 1, 10-21 (1965).
- Jaffe, S., and Klein, F.S., Trans. Far. Soc. 62, 3135-3141 (1966).
- James, T.C., and Kumer, J.B., "Fluorescence of CO₂ near 4.3 Microns: Application to Daytime Limb Radiance Calculations", J. Geophys. Res. 78, 8320-8329 (1973).
- Johnson, F.S., "Solar Radiation", Ch. 4 in F.S. Johnson, ed., Satellite Environment Handbook, Stanford University Press, Stanford (1965).
- Johnson, R., Brown, H.L., and Biondi, M.A., J. Chem. Phys. 52, 5080-5084 (1970).
- Johnston, H.S., "Gas Phase Reaction Kinetics of Neutral Oxygen Species", NSRDS-NBS 20, National Bureau of Standards (1968).
- Kasner, W.H., and Biondi, M.A., Phys. Rev. 137, A317-A329 (1965).
- Kaufman, F., Ann. Geophys. 20, 106-114 (1964).

- Kaufman, F., Can. J. Chem. 47, 1917-1924 (1969).
- Keneshea, T.J., "A Technique for Solving the Reaction Rate Equations in the Atmosphere", Environmental Research Papers No. 263, AFCRL-67-0221 (1967).
- Keneshea, T.J., and Zimmerman, S.P., J. Atm. Sci. 27, 831-840 (1970).
- Kiefer, J.H., and Lutz, R.W., "The Effect of Oxygen Atoms on the Vibrational Relaxation of Oxygen", Eleventh Symposium (International) on Combustion, pp 67-74, The Combustion Institute, Pittsburgh (1967).
- King, J.I.F., "The Source Function for an Equilibrium Gray Atmosphere", Astrophys. J. 124, 406-411 (1956).
- Krassovsky, V.I., in The Airglow and the Aurorae (ed. E.B. Armstrong and A. Dalgarno), p. 193, Pergamon Press, Oxford (1955).
- Kuhn, W.R., and London, J., J. Atmos. Sci. 26, 189-204 (1969).
- Kumer, J.B., and James, T.C., "CO₂ and N₂ Vibrational Temperatures in the $50 \leq Z \leq 130$ km Altitude Range", J. Geophys. Res. 79, 638-648 (1974).
- Lane, N.F., and Dalgarno, A., J. Geophys. Res. 74, 3011-3012 (1969).
- Lin, C.L., and Kaufman, F., "Deactivation and Reaction of N(²D)", presented at the DASA Symposium on the Physics and Chemistry of the Upper Atmosphere, Stanford Research Institute, Menlo Park, Calif. 23-24 June (1969).
- Liu, S.C., and Donahue, T.M., "Realistic Model of Hydrogen Constituents in the Lower Atmosphere and Escape Flux from the Upper Atmosphere", J. Atmos. Sci. 31, 2238-2242 (1974).
- Malkmus, W., J. Opt. Soc. Am. 58, 1214-1217 (1968).
- Malkmus, W., "Random Lorentz Band Model with Exponential Tailed S⁻¹ Line-Intensity Distribution Function", J. Opt. Soc. Am. 57, 323-329 (1967).
- Malkmus, W., "Random Band Models with Lines of Pure Doppler Shape", J. Opt. Soc. Am. 58, 1214-1217 (1968).

- Markov, M.N., Appl. Opt. 8, 887-891 (1969).
- McClatchey, R.A., Fenn, R.W., Selby, J.E.A., Garing, J.S., and Volz, F.E., "Optical Properties of the Atmosphere", Environmental Research Papers, No. 331, AFCRL-70-0527 (1970).
- Meira, L.G., Jr., J. Geophys. Res. 202-212 (1971).
- Michels, H., Harris, R., Generosa, J., and Rockwood, S., "Configuration Interaction Calculations of Electronic Transition Probabilities in Aluminum Oxide", paper presented at the DASA Symposium on Physics and Chemistry of the Upper Atmosphere, Philadelphia, Pa. 24-26 June 1970.
- Millikan, R.C., and White, D.R., Chem. Phys. 39, 3209-3212 (1963).
- Mitchell, A.C.G., and Zemansky, M.W., Resonance Radiation and Excited Atoms, Cambridge University Press, Cambridge (1961).
- Morgan, J.E., Phillips, L.F., and Schiff, H.I., Disc. Far. Soc. 33, 118-127 (1962).
- Morgan, J.E., and Schiff, H.I., Can. J. Chem. 41, 903-912 (1963).
- Nicholls, R.W., J. Res. NBS68A, 535-540 (1964a).
- Nicholls, R.W., Ann. Geophys. 20, 144-181 (1964b).
- Nicolet, M., J. Geophys. Res. 70, 679-689 (1965a).
- Nicolet, M., J. Geophys. Res. 70, 691-701 (1965b).
- Nicolet, M., Ann. Geophys. 26, 531-546 (1970).
- Norton, R.B., and Barth, C.A., J. Geophys. Res. 75, 3903-3909 (1970).
- Offerman, D., and van Zahn, U., J. Geophys. Res. 76, 2520-2522 (1971).
- Ogg, R.A., Jr., and Sutphen, W.T., J. Chem. Phys. 21, 2078 (1953).
- Ogg, R.A., Jr., and Sutphen, W.T., Disc. Far. Soc. 17, 47 (1954).
- Oppenheim, U.P., Yair Avia, and Aharon Goldman, Appl. Opt. 8, 1305-1307 (1967).
- Pearce, J.B., J. Geophys. Res. 74, 853-851 (1969a).

- Pearce, J.B., J. Quant. Spectrosc. Radiat. Transfer 9, 1593-1602 (1969b).
- Penner, S.S., Quantitative Molecular Spectroscopy and Gas Emissivities, Addison-Wesley Pub. Co., Reading, Mass. (1959).
- Roble, R.G., and Hays, P.B., Planet. Space Sci., 22, 1337-1340 (1970).
- Schiff, H.I., Can. J. Chem. 47, 1903-1916 (1969).
- Schofield, K., Planet. Space Sci. 15, 643-670 (1967).
- Schumb, W.C., Gatterfield, C.N., and Wentworth, R.L., Hydrogen Peroxide, Reinhold, N.Y. (1955).
- Schurin, B., and Clough, S.A., J. Chem. Phys. 38, 1855-1857 (1963).
- Schuring, B., and Ellis, R.E., J. Chem. Phys. 45, 2528-2532 (1966).
- Shahin, M.M., J. Chem. Phys. 47, 4392-4398 (1967).
- Shimazaki, T., and Laird, A.R., J. Geophys. Res. 75, 3221-3235 (1970).
- Simpson, C.J.S.M., Bridgman, K.B., and Chandler, T.R.D., J. Chem. Phys. 49, 509-522 (1968).
- Slanger, T.G., Wood, J. and Black, G., J. Geophys. Res. 76, 8430-8433 (1971).
- Snelling, D.R., and Bair, E.J., J. Chem. Phys. 47, 228 (1967).
- Spencer, N.W., Brace, L.H., Garignan, G.R., Taeusch, D.R., and Niemann, H., J. Geophys. Res. 70, 2665-2698 (1965).
- Stair, A.T., Jr., Ulwick, J.C., Baker, K.D., and Baker, D.J., "Rocketborne Observations of Atmospheric Infrared Emissions in the Aurora Region", to be published in Atmospheres of the Earth and Planets, ed. B.M. McCormac, D. Reidel, (1975).
- Stephenson, J.C., Wood, R.E., and Moore, C.B., J. Chem. Phys. 54, 3097-3102 (1971).
- Strobel, D.F., J. Geophys. Res. 76, 2441-2453 (1971a).
- Strobel, D.F., J. Geophys. Res. 76, 8384-8393 (1971b).

- Strobel, D.F., J. Geophys. Res. 77, 1337-1339 (1972).
- Strobel, D.F., Hunten, D.M., and McElroy, M.B., J. Geophys. Res. 75, 4307-4321 (1970).
- Taylor, R.L., and Bitterman, S., Rev. Mod. Phys. 41, 26-47 (1969).
- Taylor, R.L., Camac, M. and Feinberg, R.M., "Measurements of Vibration-Vibration Coupling in Gas Mixtures", Eleventh Symposium (International) on Combustion, pp 49-64, The Combustion Institute, Pittsburgh (1967).
- Thomas, R.J., "Total Mixing Ratios", Planet. Space Sci. 22, 175-177 (1974).
- van Tricht, C., "Asymptotic Expansions of the Integrated Absorptance for Simple Spectral Lines and Lines with Hyperfine Structure and Isotope Shifts", J. Opt. Soc. Am. 58, 669-678 (1968).
- U.S. Committee on Extension to the Standard Atmosphere, U.S. Standard Atmosphere, 1962, Government Printing Office, Wash., D.C. (1962).
- U.S. Committee on Extension to the Standard Atmosphere, U.S. Standard Atmosphere Supplements, 1966, Government Printing Office, Wash., D.C. (1966).
- Varanasi, P., and Penner, S.S., J. Quant. Spectrosc. Radiat. Transfer 7, 279-282 (1967).
- Walker, J.C.G., Planet. Space Sci. 16, 321-327 (1968).
- Walker, J.C.G., Stolarski, R.S., and Nagy, A.F., Ann. Geophys. 25, 831-839 (1969).
- Wark, D.Q., Yamamoto, G., and Lienesch, J.H., J. Atmos. Sci. 19, 369-384 (1962).
- Watanabe, K., Zelikoff, M. and Inn, E.C.Y., "Absorption Coefficients of Several Atmospheric Gases", Air Force Cambridge Research Center Report 53-23 (1953).
- Weill, G.M., " $\text{NI}(\text{S}^4\text{D})$ Radiation in the Night Airglow and Low Latitude Aurora", in B.M. McCormac and A. Omholt, eds., Atmospheric Emissions, van Nostrand Reinhold, New York (1969).

- Weller, C.S., and Biondi, M.A., Phys. Rev. 172, 198-206 (1968).
- Wofsy, S.C., McConnell, J.C., and McElroy, M.B., "Atmospheric CH₄, CO, and CO₂", J. Geophys. Res. 77, 4477-4493 (1972).
- Wofsy, S.C., and McElroy, M.B., "On Vertical Mixing in the Upper Stratosphere and Lower Mesosphere", J. Geophys. Res. 78, 2619-2624 (1973).
- Wong, E.L., and Potter, A.E., J. Chem. Phys. 43, 3371-3382 (1965).
- Wray, K.L., and Teare, J.D., J. Chem. Phys. 36, 2582-2596 (1962).
- Yardley, J.T., J. Chem. Phys. 49, 2816-2821 (1968).
- Zelikoff, M., Watanabe, K., and Inn, E.C.Y., J. Chem. Phys. 21, 1643 (1953).

APPENDIX

CHEMISTRY PROGRAM SNAPS2

The chemistry program developed by Degges (1972) is listed here for reference purposes. Its main use has been to estimate diurnal variations in chemical abundances, given initial molecular species concentrations.

The reaction rates originally used are listed in Table A-1. The new values of Garvin and Hampson (1974) are listed in Table A-2 when the values vary by fifty per cent or more.

The chemistry program consists of a main program, SNAPS2, and 6 subroutines; ROMTST, TKEL, SOLLY, CONCEN, COLUMN, and SUNPHI. The main program performs the chemical computations, including the effects of vertical transport. ROMTST embodies the extrapolation method of Bulirsch and Stoer (1966). TKEL is used to compute temperatures at each altitude. SOLLY computes the solar zenith angle and fraction of the solar disk visible at each altitude. COLUMN integrates the number densities of molecular nitrogen, oxygen and ozone above a given altitude in the direction of the sun. CONCEN is called by COLUMN to obtain number densities required for the integration. SUNPHI computes the attenuation of solar flux by absorption between a given altitude and the assumed top of the atmosphere in the solar direction and returns the photodissociation rates required for the chemistry.

The operation of the main program is described briefly below.

Preceding page blank

Table A-1

Reaction Rates for Neutral Species

Reactants and products are in lowest electronic state unless indicated explicitly.
Where two rates are given, (a) is for the reaction as written, (b) is for the reverse.

	<u>Reaction</u>	<u>Rate Coefficient, c.g.s. units</u>	<u>Source</u>	<u>Error Estimate</u>
R1a	$O + O + M \rightarrow O_2 + M$	$3.8 \times 10^{-30} T^{-1} \exp(-171/T)$	Johnston (1968)	High by up to 50%
R1b		$4.57 \times 10^{-5} T^{-1} \exp(-59700/T)$	Johnston (1968)	30%
R2a	$O + O_2 + M \rightarrow O_3 + M$	$4.63 \times 10^{-35} \exp(1060/T)$	Johnston (1968)	30%
R2b		$1.65 \times 10^{-9} \exp(-11920/T)$	Johnston (1968)	30%
R3a	$O + O_3 \rightarrow 2O_2$	$2.0 \times 10^{-11} \exp(-2410/T)$	Johnston (1968)	30%
R3b		$2.12 \times 10^{-11} \exp(-50700/T)$	Johnston (1968)	30%
R4	$H + O_3 \rightarrow OH + O_2$	2.6×10^{-11}	Kaufman (1969)	20% at 300 K
R5a	$O + OH \rightarrow H + O_2$	2.06×10^{-11}	Schofield (1967)	50%
R5b		$4.19 \times 10^{-10} \exp(-8450/T)$	Schofield (1967)	50%
R6	$O + HO_2 \rightarrow OH + O_2$	$\geq 10^{-11}$	Kaufman (1969)	
R7	$H + HO_2 \rightarrow H_2O + O$	$2.0 \times 10^{-10} \exp(-2000/T)$	Bates and Nicolot (1950)	An estimate
R8	$H + O_2 + M \rightarrow HO_2 + M$	$3.0 \times 10^{-32} (273/T)^{1.3}$	Schofield (1967)	30%

	<u>Reaction</u>	<u>Rate Coefficient, c.g.s. units</u>	<u>Source</u>	<u>Error Estimate</u>
R9	$\text{OH} + \text{O}_3 \rightarrow \text{HO}_2 + \text{O}_2$	$\leq 5.0 \times 10^{-13}$	Kaufman (1969)	
R10	$\text{HO}_2 + \text{O}_3 \rightarrow \text{OH} + 2\text{O}_2$	10^{-14}	Hunt (1964)	An estimate
R11a	$\text{OH} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{O}$	$9.3 \times 10^{-12} \exp(-390/T)$	Baulch, et al. (1968b)	20% at 300 K
R11b		$9.3 \times 10^{-11} \exp(-9000/T)$	Baulch, et al. (1968b)	20% at 300 K
R12	$\text{OH} + \text{HO}_2 \rightarrow \text{H}_2\text{O} + \text{O}_2$	$\geq 10^{-11}$	Kaufman (1969)	See Text
R13	$\text{H} + \text{HO}_2 \rightarrow \text{H}_2 + \text{O}_2$	2.0×10^{-13}	Clyne and Thrush (1963)	30%
R14	$\text{O} + \text{H}_2 \rightarrow \text{OH} + \text{H}$	$7.0 \times 10^{-11} \exp(-5100/T)$	Wong and Potter (1965)	30%
R15	$\text{HO}_2 + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{O}_2$	1.5×10^{-12}	Kaufman (1969)	30%
R16	$\text{OH} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2\text{O} + \text{HO}_2$	4.0×10^{-13}	Foner and Hudson (1962)	50%
R17	$\text{O} + \text{H}_2\text{O}_2 \rightarrow \text{OH} + \text{HO}_2$	10^{-15}	Foner and Hudson (1962)	50%
R18	$\text{H} + \text{H}_2\text{O}_2 \rightarrow \text{H}_2 + \text{HO}_2$	10^{-13}	Foner and Hudson (1962)	50%
R19a	$\text{OH} + \text{H}_2 \rightarrow \text{H}_2\text{O} + \text{H}$	$* 3.6 \times 10^{-11} \exp(-2600/T)$	Baulch, et al. (1968b)	35% at 300K
R19b		$* 1.4 \times 10^{-10} \exp(-10100/T)$	Baulch, et al. (1968b)	35% at 300 K
R20	$\text{O} + \text{H} + \text{M} \rightarrow \text{OH} + \text{M}$	$* 8.0 \times 10^{-33}$	Bates and Nicolet (1950)	Estimate
R21	$\text{O} + \text{OH} + \text{M} \rightarrow \text{HO}_2 + \text{M}$	$* 1.4 \times 10^{-31}$	Kaufman (1964)	30%

	<u>Reaction</u>	<u>Rate Coefficient, c.g.s. units</u>	<u>Source</u>	<u>Error Estimate</u>
R22	$H + H + M \rightarrow H_2 + M$	$* 1.2 \times 10^{-32} (273/T)^{0.7}$	Kaufman (1969)	30%
R23	$H + OH + M \rightarrow H_2O + M$	$* 2.5 \times 10^{-31}$	Kaufman (1964)	50%
R24	$H + HO_2 \rightarrow 2OH$	$* \geq 3 \times 10^{-12}$	Kaufman (1969)	
R25	$H + HO_2 \rightarrow H_2 + O_2$	$* \geq 3 \times 10^{-12}$	Kaufman (1969)	
R26	$H + OH \rightarrow H_2 + O$	$* 3.0 \times 10^{-11} \exp(-4170/T)$	Kaufman (1969)	30%
R27	$O(^1D) + N_2 \rightarrow O(^3P) + N_2$	5.0×10^{-11}	Donovan and Husain (1970)	50%
R28	$O(^1D) + O_3 \rightarrow O_2 + O_2$	5.0×10^{-11}	Snelling and Bair (1969)	50%
R29	$O(^1D) + H_2 \rightarrow OH + H$	1.0×10^{-11}	Donovan and Husain (1970)	Uncertain
R30	$O(^1D) + H_2O \rightarrow OH + OH$	3.0×10^{-11}	Donovan and Husain (1970)	Uncertain
R31	$O(^1D) + H_2O \rightarrow OH + OH$	$* 10^{-11}$	Estimate	
R32	$O(^1D) + CH_4 \rightarrow \text{Products}$	10^{-11}	Donovan and Husain (1970)	Uncertain
R33	$CO + OH \rightarrow CO_2 + H$	$1.0 \times 10^{-12} \exp(-540/T)$	Baulch, et al. (1968a)	30%
R34	$CO + O + M \rightarrow CO_2 + M$	$1.4 \times 10^{-33} \exp(-1250/T)$	Baulch, et al. (1968a)	Extremely uncertain
R35	$CO + HO_2 \rightarrow CO_2 + OH$	$* 2.5 \times 10^{-17}$	Schofield (1967)	Uncertain
R36	$CH_4 + OH \rightarrow H_2O + CH_3$	$1.2 \times 10^{-10} \exp(-2960/T)$	Schofield (1967)	30%
R37	$O + CH_4 \rightarrow OH + CH_3$	$3.5 \times 10^{-11} \exp(-4550/T)$	Herron (1969)	50%

	<u>Reaction</u>	<u>Rate Coefficient, c.g.s. units</u>	<u>Source</u>	<u>Error Estimate</u>
R38	$\text{CH}_3 + \text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{OH}$	$*5.0 \times 10^{-11} \exp(-5000/\text{T})$	Dean and Kistiakowski (1971)	Uncertain
R39	$\text{CH}_2\text{O} + \text{OH} \rightarrow \text{H}_2\text{O} + \text{HCO}$	$*5.3 \times 10^{-10} \exp(-2120/\text{T})$	Schofield (1967)	50%
R40	$\text{CH}_2\text{O} + \text{HO}_2 \rightarrow \text{H}_2\text{O}_2 + \text{HCO}$	$*7.5 \times 10^{-15}$	Schofield (1967)	Uncertain
R41	$\text{HCO} + \text{O}_2 \rightarrow \text{CO} + \text{HO}_2$	$*1.0 \times 10^{-13}$	Estimate	Uncertain
R42a	$\text{N} + \text{O}_2 \rightarrow \text{NO} + \text{O}$	$1.1 \times 10^{-14} \text{T} \exp(-3140/\text{T})$	Baulch, et al. (1969)	30% at 300 K
R42b		$2.6 \times 10^{-15} \text{T} \exp(-19500/\text{T})$	Baulch, et al. (1969)	30%
R43a	$\text{N} + \text{NO} \rightarrow \text{N}_2 + \text{O}$	$5.1 \times 10^{-11} \exp(-168/\text{T})$	Baulch, et al. (1969)	Factor of 2
R43b		$2.3 \times 10^{-10} \exp(-37500/\text{T})$	Baulch, et al. (1969)	Factor of 2
R44a	$\text{NO} + \text{NO} \rightarrow \text{N}_2 + \text{O}_2$	$1.3 \text{T}^{-5/2} \exp(-42800/\text{T})$	Freedman and Daiber (1961)	Highly uncertain
R44b		$15.2 \text{T}^{-5/2} \exp(-64300/\text{T})$	Wray and Teare (1962)	Highly uncertain
R45	$\text{N} + \text{N} + \text{M} \rightarrow \text{N}_2 + \text{M}$	$1.4 \times 10^{-33} \exp(-500/\text{T})$	Schiff (1969)	Factor of 2
R46a	$\text{N} + \text{O} + \text{M} \rightarrow \text{NO} + \text{M}$	$1.1 \times 10^{-32} (273/\text{T})^{1/2}$	Baulch, et al. (1969)	50%
R46b		$3.8 \times 10^{-7} \text{T}^{-1/2} \exp(-74500/\text{T})$	Baulch, et al. (1969)	Factor of 5
R47	$\text{O} + \text{NO} \rightarrow \text{NO}_2 + \text{h}\nu$	$6.5 \times 10^{-17} (\text{T}/296)$	Baulch, et al. (1970)	Factor of 2
R48	$\text{O} + \text{NO}_2 \rightarrow \text{NO} + \text{O}_2$	$1.6 \times 10^{-11} \exp(-300/\text{T})$	Baulch, et al. (1970)	20%

	<u>Reaction</u>	<u>Rate Coefficient, c.g.s. units</u>	<u>Source</u>	<u>Error Estimate</u>
R49	$N + NO_2 \rightarrow N_2O + O$	$*7.8 \times 10^{-12}$	Schiff (1969)	30% at 300 K
R50	$N + NO_2 \rightarrow N_2 + 2O$	2.3×10^{-12}	Schiff (1969)	Factor of 2 at 300 K
R51	$N + NO_2 \rightarrow N_2 + O_2$	$*1.8 \times 10^{-12}$	Schiff (1969)	Factor of 2 at 300 K
R52	$N + NO_2 \rightarrow 2NO$	5.9×10^{-12}	Schiff (1969)	30% at 300K
R53a	$NO + O + M \rightarrow NO_2 + M$	$2.9 \times 10^{-33} \exp(940/T)$	Baulch, et al. (1970)	20%
R53b		$1.8 \times 10^{-8} \exp(-32800/T)$	Baulch, et al. (1970)	25% at 1500 K
R54a	$NO + NO + O_2 \rightarrow NO_2 + NO_2$	$6.6 \times 10^{-39} \exp(530/T)$	Baulch, et al. (1970)	50%
R54b		$6.6 \times 10^{-12} \exp(-13500/T)$	Baulch, et al. (1970)	50%
R55	$O_3 + NO \rightarrow NO_2 + O_2$	$9.5 \times 10^{-13} \exp(-1240/T)$	Schiff (1969)	30%
R56	$N + O_2(\Delta_g) \rightarrow NO + O$	$*3.0 \times 10^{-15}$	Clark and Wayne (1969)	30%
R57	$N + O_3 \rightarrow NO + O_2$	$*3.0 \times 10^{-11} \exp(-1200/T)$	Nicolet (1965)	An estimate
R58	$N(^2D) + O_2 \rightarrow NO + O$	6.0×10^{-12}	Lin and Kaufman (1969)	20% at 300 K
R59	$N(^2D) + N_2O \rightarrow NO + N_2$	$*3.6 \times 10^{-13} T^{1/2} \exp(-400/T)$	Slanger, et al. (1971)	50%
R60	$N + OH \rightarrow NO + H$	$*6.8 \times 10^{-11}$	Campbell and Thrush (1968)	20% at 320 K
R61	$N(^2D) + O \rightarrow N(^4S) + O$	2.0×10^{-13}	Weill (1969)	An estimate

*An asterisk preceding the rate coefficient indicates that the reaction is not included in the present version of the chemistry program.

Table A-2
Revised Values for Reaction Rates
From Garvin and Hampson (1974)

R5a	4.2×10^{-11}
R6	$8.0 \times 10^{-11} \exp (-500/T)$
R8	$6.7 \times 10^{-33} \exp (+290/T)$
R9	$1.6 \times 10^{-12} \exp (-1000/T)$
R10	$1.0 \times 10^{-13} \exp (-1250/T)$
R12	should vary between 2×10^{-11} and 2×10^{-12}
R13	$4.2 \times 10^{-11} \exp (-350/T)$
R14	$3.0 \times 10^{-14} \exp (-4480/T)$
R15	$3.0 \times 10^{-11} \exp (-500/T)$
R16	$1.7 \times 10^{-11} \exp (-910/T)$
R17	$2.8 \times 10^{-12} \exp (-2125/T)$
R18	$2.8 \times 10^{-12} \exp (-1900/T)$
R29	2.9×10^{-16}
R30	3.5×10^{-10}
R33	1.4×10^{-13}
R36	$3.0 \times 10^{-12} \exp (-1770/T)$
R47	6.5×10^{-17}
R48	9.1×10^{-12}
R57	5.7×10^{-13}

Table A-3

Photodissociation Processes Considered for Chemistry Program

	Reaction	Source of Cross Sections
J1	$O_2 + h\nu \rightarrow O(^3P) + O(^3P)$	Hudson, Carter and Breig (1969) Ackerman (1970)
J2	$O_2 + h\nu \rightarrow O(^1D) + O(^3P)$	Ackerman (1970)
J3	$O_3 + h\nu \rightarrow O(^3P) + O_2$	Ackerman (1970)
J4	$O_3 + h\nu \rightarrow O(^1D) + O_2$	Ackerman (1970)
J5	$H_2O + h\nu \rightarrow OH + H$	Watanabe, et al. (1953)
J6	$H_2O_2 + h\nu \rightarrow OH + OH$	Schumb, et al. (1955)
J7	$HO_2 + h\nu \rightarrow OH + O(^3P)$	Assumed same as H_2O_2
J8	$NO + h\nu \rightarrow NO^+ + e$	Donahue (1966)
J9	$NO_2 + h\nu \rightarrow NO + O(^3P)$	Hall and Blacet (1952)
J10	$NO_2 + h\nu \rightarrow N(^4S) + O_2$	Strobel (1971b)
J11	$N_2O + h\nu \rightarrow NO + N(^4S)$	Zelikoff, et al. (1953)
J12	$N_2 + h\nu \rightarrow 2N(^4S)$	Hudson and Carter (1969)
J13	$CO_2 + h\nu \rightarrow CO + O$	Watanabe, et al. (1953)
J14	$CH_4 + h\nu \rightarrow CH_3 + H$	Watanabe, et al. (1953)

Solar fluxes for Lyman- α (1216 Å) and wavelengths longer than 1170 Å were taken from Ackerman (1970). Selection of cross section data was aided by the review of Hudson (1971).

Program Flow:

Execution of Program SNAPS begins with the initialization of constants used by the program. The values of eddy diffusion coefficients used at altitudes above 40 km are stored in array EDCOEF. The peak value set by the DATA statement occurs at 104 km. The eddy diffusion coefficient profile is lowered by 9 km in the DO loop ending with statement 90 and the low altitude eddy diffusion coefficients in array EDCF are transferred to array EDCOEF in the DO loop ending with statement 95. This permits use of separate sets of high and low altitude diffusion coefficients by changing the appropriate data statements, and easy variation of the altitude of maximum turbulent transport. The data described above is then read in. The information on each data card is written to printer output channel 6 as it is read. Columns 13 through 80 of the second through fourteenth data cards are printed in addition to the number placed in columns 2 through 12 so that comments may be added. The first 14 data cards are printed on a page numbered -1. The input concentrations require about 10 pages to print, the first of which is numbered page 0. Further execution is determined by the input data. A brief flow chart is given on the next page.

The outermost control DO loop ending with statement 450 is executed IHRMAX times. Within this loop, the computer clock is called and computer running time since the beginning of the program is stored in variable SECA. Variable locations used in the DO loop ending with statement 110 are set to zero and this loop is entered and executed for each altitude between NBASE and NTOP.

The mean molecular mass RMWT at each altitude is computed by the statements associated with DO loop 102. Temperatures are computed by calls to function TKEL. The gravitational acceleration at each altitude is computed and local mixing scale heights H_{av} are computed. Coefficients for the eddy diffusion contributions to g and β terms in Equation (3-4) are determined from a finite difference approximation, and stored in arrays BTED, QJEDL and QJEDU. Factors needed for computation of molecular diffusion contributions are computed and stored in arrays AFAC, BFAC, CFAC, DFAC and RDTEMP. The molecular concentrations at each altitude above the base altitude are scaled to be consistent with the finite difference scheme in the DO loop ending with statement 104. An effective molecular scale temperature is used for the local scale height. Before exit from DO loop 110, N_2 and O_2 concentrations and sample computed values are written to the printer output channel for altitudes between but not including those associated with NBASE and NTOP.

The DO loop ending with statement 400 is entered and executed MMAX times. Each execution advances the integration time by DLTIME seconds. The time at the end of the step is computed in floating and fixed point form. If the value of NPRNT permits, a new page is started and the time and column headings are printed. Molecular diffusion coefficients are computed for the two lowest altitudes in the statements associated with DO loop 130.

The DO loop ending with statement 350 is entered and executed for each altitude. Molecular diffusion coefficients are computed for the next higher altitude, and the molecular diffusion contributions to the β and g terms are computed and combined with the eddy diffusion contributions in the DO loop ending with statement 140. The solar zenith angle CHI and the fraction ETA of the sun's disc visible are computed by Subroutine SOLLY. If the sun is visible, column counts of N_2 , O_2 , O and O_3 in the solar direction are computed in Subroutine COLUMN and photodissociation rates are computed in Subroutine SUNPHI for the time at the midpoint of the time interval of integration. Reaction rate coefficients are computed for the temperature at the given altitude.

The integration for a global time increment DLTIME at a single altitude is performed in the DO loop ending with statement 300. The operations within this loop are repeated either until convergence to relative accuracy EPS is achieved or until MLMAX repetitions have been performed with no convergence. Each time through this loop, a new number of local time intervals, MMF, is computed to conform to the extrapolation procedure of Subroutine ROMTST. Values of the initial concentrations at the integration altitude in array CONSP are placed in array DCX. The DO loop ending with statement 290 then integrates over the MMF local time steps. The values in array DCX are copied into array TCX and the time increment DTIME is set to one-half the length of the local

increment. An index ITER is set to one and appropriate third body concentrations are computed. The algorithm of Equation 2-10 is then applied for each species in the DO loop ending with statement 255, the results being placed in array RCX. ITER is incremented and the results in array RCX are placed in array TCX. The time increment is doubled and the DO loop ending with statement 255 is again executed, using the intermediate results from the first execution to compute the α , β and g terms. The results of this second cycle, computed in array RCX, are transferred to array DCX and the statements in the DO loop ending with statement 290 repeated until the global time interval DLTIME has been covered. Subroutine ROMTST is called to test the values in array DCX with previous results produced in the DO range ending with statement 290. The improved concentration values are returned in array TCX. If convergence is achieved, control is transferred to statement 310. Otherwise, the DO loop ending with statement 300 is repeated. If this process does not result in convergence in MLMAX tries, the end point values in array RCX are placed in array TCX in the DO loop ending with statement 315. The endpoint results for the next lower altitude, which have been stored in array SCX, are written into array CONSP and the contents of array TCX are placed in array SCX. Production rates for OH by two different reactions are computed and stored in QCOHA and QCOHB. "Rectangular" sums of total column counts are incremented in DZOHA and DZOHB. These values are computed to

provide a rough check on the hydrogen compound chemistry and may be compared with airglow observations. If the value of NPRNT permits, the altitude, QCOHA, QCOHB, DZOHA, DZOHB and the concentrations of 16 molecules are written to the printer output channel. The statements in the DO loop ending with statement 350 are then repeated until concentrations at all altitudes between (but not including) NBASE and NTOP have been integrated over the global time step DLTIME.

When all altitudes have been integrated, a summary of number of iterations is sent to the printer output channel and the time value TIME is incremented by DLTIME.

After the integration has been advanced MMAX times with time increment DLTIME, all concentrations are sent to the punch output channel by the statements in DO loop 420 and to the printer channel by the statements in DO loop 440. The internal computer clock is again accessed and the starting, end, and elapsed time required in DO loop 450 are sent to the printer output channel. Program execution ceases after this outer DO loop has been executed IHRMAX times.

The scaling of concentrations performed in the DO loop ending with statement 104 permits use of output data from runs at another latitude or with a different temperature profile to be used as input data. While there may be some difficulty in reaching convergence at altitudes below 90 km in the first time step, this is not a serious problem. When using a global time step DLTIME of 600 seconds and a value of 0.01 for EPS, computation of chemical changes

over a day for 150 altitudes requires on the order of 20 minutes running time on the CDC 6600. This is longer than would be required by the differencing methods usually employed (e.g., Shimazaka and Laird, 1970) but the error control compensates for this. It is not necessary to alter time increments at dawn or sunset since the convergence algorithm of Subroutine ROMTST automatically forces the use of smaller time subdivisions of the global time interval DLTIME.

Inputs:

The necessary input data to the chemistry program is a set of 14 data cards containing identification and variable parameters and a set of 603 cards containing concentrations of N_2 , O_2 , $O(^3P)$, O_3 , OH , H , H_2O , HO_2 , H_2O_2 , H_2 , CH_4 , CO_2 , CO , $O(^1D)$, $N(^4S)$, NO , NO_2 , N_2O , $N(^2D)$ and Ar at one km intervals between ground level and 200 km. The data is read in the following order:

1. IDENT 60 characters of identifying comments which are used in output page headings. The first character should be a blank.
2. DTHETA Co-latitude, degrees, of the computation location. A value of zero corresponds to the north pole.
3. DPH1 East longitude, degrees, of computation location.
4. SOLDEC Solar declination angle, degrees, used to determine time of year.
5. GREF Surface gravitational acceleration, cm/sec^2 , at computation location.

- | | |
|------------|---|
| 6. REFF | Effective value of earth radius, km, for use in computing gravitational accelerations at points above ground level. |
| 7. EPS | Relative error permitted for each time step in the integration. |
| 8. MLMAX | Maximum number of times integration is to be attempted for each time step to obtain relative error EPS. |
| 9. NBASE | Index of base altitude for computations, altitude in km plus one. |
| 10. NTOF | Index of highest altitude in computations, altitude in km plus one, restricted to 201 or less in current program. |
| 11. IHRMAX | Number of times at which complete output is required. |
| 12. MMAX | Number of integration steps between complete output points. |
| 13. DLTIME | Integration interval, seconds; the total simulated time for a given run, in seconds, is $IHRMAX * MMAX * DLTIME$. |
| 14. TIME | Initial time, seconds, measured from noon; AM values are negative, PM values are positive. |
| 15. CONSP | The 603 cards containing concentrations and identifying indices; concentrations are read into array CONSP. |

Outputs:

A complete set of data, identical to the input data, is written on tape 4 at the end of each major time step.

Mnemonic Variables:

Real Arrays: AFAC

Stores values of numerical approximation to $\frac{1}{T} \frac{\partial T}{\partial z}$.

AMWT

Stores values of molecular weights, gm/mole; values are set by data statement.

BFAC

Stores values of the coefficient of molecular concentration in the numerical approximation to $-\left[\frac{\partial^2 n}{\partial z^2} + \frac{1}{T} \frac{\partial^2 T}{\partial z^2} n - \frac{1}{T^2} \left(\frac{\partial T}{\partial z}\right)^2\right]$

BTED

Stores values of coefficients used in computing contribution to β terms from eddy diffusion.

BTEMD

Stores values of contribution to β term from both eddy and molecular diffusion for each molecule at a given altitude during integration.

CARD

Used as temporary storage for comments in columns 13 through 80 of first 14 data cards.

CFAC

Stores values of numerical approximation used to compute $\frac{1}{H^2} \frac{\partial H}{\partial z}$ for diffusive scale heights.

CMD

Stores values of molecular diffusion coefficients for each molecular species at a given altitude during integration.

CMDL

Stores values of CMD at next lower altitude.

CMDU

Stores values of CMD at next higher altitude.

COL

Stores values of integrated column counts computed by Subroutine COLUMN.

CONSP	Stores values of molecular number densities; initial values are read in from cards; values are altered at each integration step.
DCX	Stores initial number densities for one altitude during local time step in integration.
DFAC	Stores values of g/RT used in computing atmospheric scale heights and contribution of molecular diffusion.
EDCF	Stores values of eddy diffusion coefficients for altitudes below 40 km, set by DATA statement.
EDCOEF	Stores values of eddy diffusion coefficients, initially contains high altitude values set by DATA statement.
QJEDL	Stores coefficients of eddy diffusion contribution to g terms from next lower altitude.
QJEDU	Stores coefficients of eddy diffusion contributions to g terms from next higher altitude.
QJEMD	Stores values of contribution to g term from eddy and molecular diffusion for each molecular species at a given altitude during integration.
RATE	Stores values of photodissociation rates computed by Subroutine SUNPHI.
RCX	Stores intermediate values of number densities for a single altitude computed during local time step in integration.

RDTEMP	Stores values of temperature coefficients used in computing molecular diffusion coefficients.
SCX	Stores values of number densities computed at end of global time step for next lower altitude; values eventually replace corresponding numbers in CONSP.
TCX	Stores intermediate values of number densities used in computing α , β and g values during integration of local time step for a single altitude.
TEMPK	Stores values of temperatures at each altitude, values are computed by function TKEL.
TETOT	Stores values of total electron densities at each altitude, values are set by DATA statement.
TFMT	Stores format statement for computer running time printout, set by DATA statement.
TINO	Stores values of NO^+ concentrations at each altitude, set by DATA statement.
TIO	Stores values of O^+ concentrations at each altitude, set by DATA statement.
TIO2	Stores values of O_2^+ concentrations at each altitude, set by DATA statement.
TST	Used as workspace by Subroutine ROMTST.

The names of integer arrays and their uses are:

IDENT	Stores 60 character comment read from
-------	---------------------------------------

	first data card, which is used in page headings.
IDNT	Stores image of last 20 characters of first data card.
LSP	Stores Hollerith constants used in printing column headings.
MLPRNT	Stores data on number of iterations required for convergence of integration at a given altitude, and (largest) index of species which did not converge in MLMAX iterations.

Real Variables:

AFACNA	Temporary storage of value of AFAC for altitude at which integration is being performed.
BFACNA	Temporary storage of value of BFAC for altitude at which integration is being performed.
BTEDNA	Temporary storage of value of BTED for altitude at which integration is being performed.
BTSQ	Square of β term used in integration.
BTT	Value (partial or complete) of β term used in integration for a single molecular species.
CFACNA	Temporary storage of value of CFAC for altitude at which integration is being performed.
CHI	Solar zenith angle, radiance, computed by Subroutine SOLLY.

CHISAV	Temporary storage for value of CHI.
CMDNSP	Temporary storage for value of molecular diffusion coefficient for single molecular species.
CON	Temporary storage for factor used in scaling molecular concentrations at altitude NTOP to fit scale height defined by molecular scale temperature.
CONFAC	Temporary storage for factor used to scale molecular concentrations to fit local scale heights defined by molecular scale temperature.
CONSPN	Temporary storage for concentration of a single molecular species at a given altitude.
C1	Temporary storage for molecular nitrogen concentration.
C2	Temporary storage for molecular oxygen concentration.
C3	Temporary storage for atomic oxygen concentration.
DCT	Temporary storage for single value from array DCX.
DDDZ	Temporary storage for value of $\frac{\partial D}{\partial z}$ for single molecular species.
DELZ	Altitude increment, cm.
DFACNA	Temporary storage for value of DFAC at altitude for which integration is being performed.
DHDZ	Temporary storage for value of $\frac{\partial H}{\partial z}$.
DKDZ	Temporary storage for value of $\frac{\partial K}{\partial z}$.

DLT	Value of δ used in integration for a single molecular species.
DLTIME	Time increment for integration step, read in as data.
DPHI	East longitude of point of integration, read in as data; not needed in present program which assumes times are true solar times.
DTDZ	Temporary storage for value of $\frac{\partial T}{\partial z}$.
DTHETA	Colatitude of point at which integration is performed, read in as data.
DTIME	Storage for value of local time step in integration.
DZOHA } DZOHB }	Values of integrated production rates of OH.
ED	Temporary storage for value of eddy diffusion coefficient at a given altitude.
EPS	Value of relative error allowed in integration.
ETA	Fraction of solar disc visible at given altitude.
FAC	Temporary storage for intermediate results, use varies in different parts of program.
FACB	Temporary storage for either βt or δt in Equations (2-10).
FACDMB	Temporary storage for $\delta - \beta$ in Equatio (3-5).
FACM	Temporary storage for value of $1 - \exp(-\delta t)$.
FACRT	Temporary storage for $4 \propto g / \beta^2$.
FAC2AX	Temporary storage for $2 \propto x$.
FAC4AQ	Temporary storage for $4 \propto g$.
G	Value of graviational acceleration at altitude NALT.

GL	Value of graviational acceleration at altitude NALT -1.
GRES	Surface value of graviational acceleration, read in as data.
GU	Value of graviational acceleration at altitude NALT +1.
QCOHA	Values of OH production rates at altitude of integration.
QCOHB	
QJEDLN	
	Temporary storage for value of QJEDL at altitude of integration.
QJEDUN	Temporary storage for value of QJEDU at altitude of integration.
QJT	Temporary storage for partial or complete value of g term used in integration of a single molecular species.
RDELZ	Reciprocal of twice the altitude increment DELZ.
RE	Effective radius of earth, km, used in geometrical computations.
REFF	Effective radius of earth, km, used in gravitational calculations, read in as data.
RFAC	Temporary storage of intermediate results.
RI1, ...	Storage for values of ionic reaction rates.
RMWT	Mean molecular mass at altitude NALT.
RMWTL	Mean molecular mass at altitude NALT -1.
RMWTU	Mean molecular mass at altitude NALT +1.
ROBS	Altitude of given point, km.
RTIME	Variable used in printing time values.
RI, ...	Values of forward neutral reaction rates.
R2DELZ	Square of reciprocal of altitude increment, DELZ.

SECA	}	Storage for values of computation of computer running time.
SECB		
SECC		
SFAC		Temporary storage of intermediate results.
SH		Value of mixing scale height at altitude NALT.
SHL		Value of mixing scale height at altitude NALT -1.
SHU		Value of mixing scale height at altitude NALT +1.
SII, ...		Values of reverse ionic reaction rates.
SOLDEC		Solar declination angle, read in as data.
SUM	}	Temporary storage used in forming mean molecular masses.
SUML		
SUMU		
SI, ...		Values of reverse neutral reaction rate coefficients.
TCH4, ...		Values of individual molecular concentrations in array TCX, named individually for convenience in forming α , β and g coefficients. TCH4 corresponds to CH ₄ , TCO corresponds to CO, etc.
TEMP		Value of temperature at altitude NALT.
TEMPI		Reciprocal of temperature.
TEMPL		Value of temperature at altitude NALT - 1.
TEMPU		Value of temperature at altitude NALT +1.
TEMP12		Value of minus one-half power of temperature.
TEMP32		Value of minus three-halves power of temperature.

TEMP52	Value of minus five-halves power of temperature.
TFAC	Temporary storage of intermediate results.
TIME	Time, expressed in seconds from noon, read in as data; altered in program to be the time at midpoint of a global integration step so that approximate mean values of photodissociation rates will be computed by Subroutine SUNPHI.
XM4,...	Third body concentrations for appropriate three-body reactions.
XXX12	Storage for factor used in computing g term for CO_2 and β term for CO.

Integer Variables:

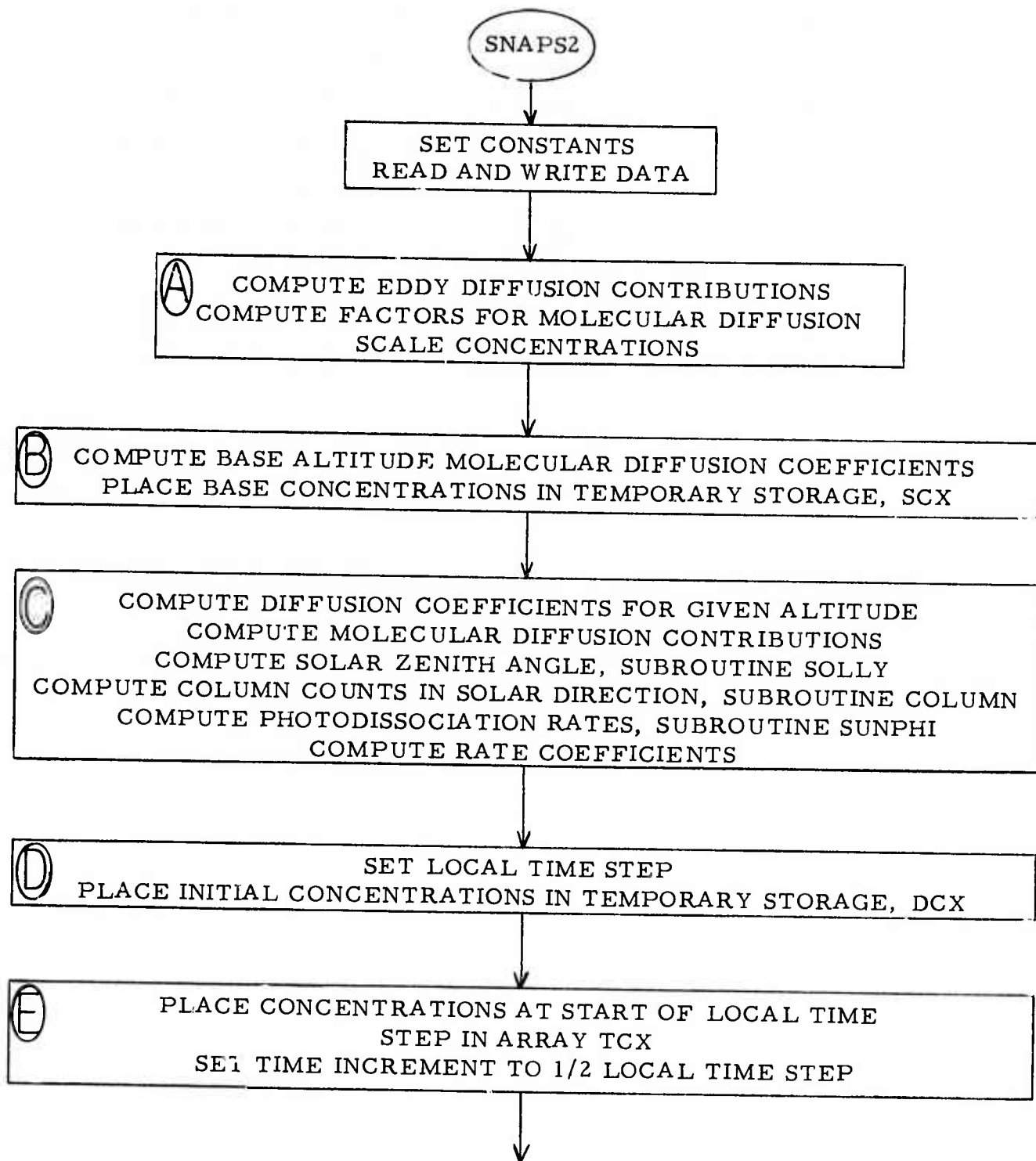
I	Index in DO loop 95, auxiliary index in DO loop 110, and index in implied input/output DO loops.
IF	Final parameter in innermost implied DO loop used in printing output concentrations within DO loop 440.
IHR	Index in DO loop 450.
IHRMAX	Final parameter in DO loop 450, input as data.
IP	Index in print control DO loop 440.
IS	Initial parameter in implied DO loop, see IF.
ITER	Control index in integration, used between statements 200 and 260 to select proper values for array TCX.

IX	Index in DO loop 435, incremented for each page of output.
J	Index in implied DO loops used in reading data into array CONSP within DO loop 100.
KCH4, ...	Index variables used to select appropriate values of quantities related to given species; most uses replaced by use of TCH4, etc.
KTEST	Parameter returned by Subroutine ROMTST, zero if integration has converged, non-zero otherwise.
LALT, LCHI, LCOLN2, LCOLO2, LCOLO3, LDZOHA, LDZOHB, LJO2, LJO3, LML, LQCOHA, LQCOHB, LTIME	Store Hollerith constants used in printing column headings and are set by DATA statements.
M	Index of DO loop 400, incremented for each global time step.
ML	Index of DO loop 300, incremented for each iteration of integration over global time step at a given altitude.
MLMAX	Final parameter of DO loop 300, read in as data.
MLSAVE	Temporary storage for value of ML, used after exit from DO loop 300 to print number of iterations required for convergence.
MMAX	Final parameter of DO loop 400, read in as data.
MMF	Final parameter of DO loop 290, computed from ML and is number of local subdivisions of global time step DLTIME for the ML iteration of integration.

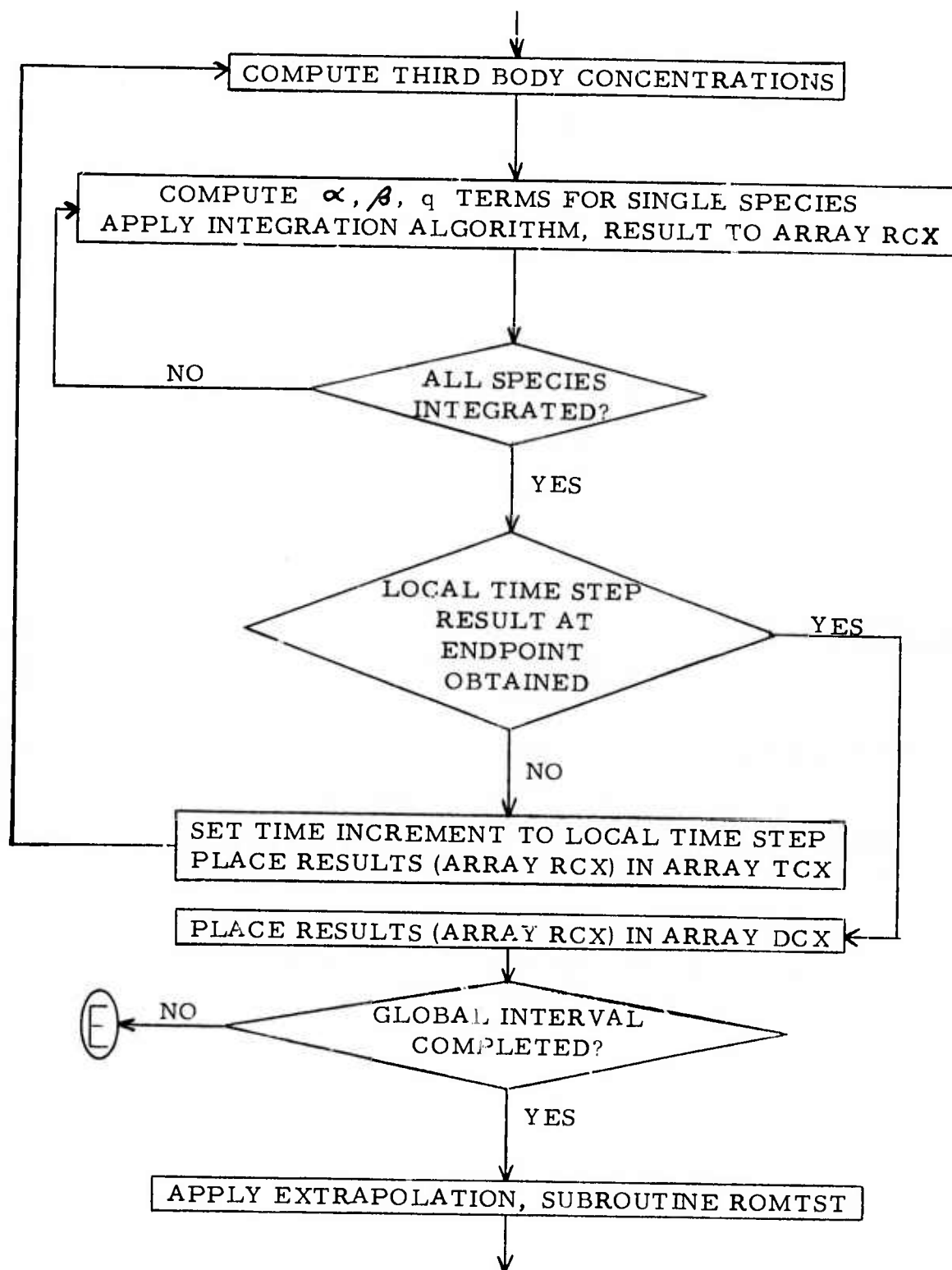
MMS	Index for DO loop 290, see MMF.
NA	Auxiliary index, usually set to NALT -1.
NALT	Index for DO loops 90, 100, 110, 350, 420 and 430; denotes a given altitude.
NAMIN	Value of NALT -1 in DO loop 350.
NB	Value of NALT -2 in DO loop 110.
NBASE	Index of lowest altitude for integration, read in as data.
NF	Final parameter of DO loop 430.
NMIN	Stores input value of NBASE, which is changed by program.
NPAGE	Stores output page number.
NPLU	Value of NALT +1 in DO loop 350.
NPRNT	Variable available to control output of concentrations at integration steps intermediate to fully documented output at end of DO loop 450, set to 1 at present, so values are output for each interval DLTIME.
NS	Initial parameter of DO loop 430.
NSP	Index in DO loops 102, 104, 130, 140, 180, 190, 255, 258, 280, 315, and 320; a value of NSP selects a value of a variable corresponding to a single molecular species.
NSPM	Number of molecular species included in program, 20 at present, used as final parameter of DO loops with NSP as index.
NT	Final parameter of DO loop 420, in which output cards are punched.

NTIME	Used in printing time values.
NTOP	Index of highest altitude used in integration, input as data.
NW	Channel number for printing computer running time information, set to 6 here.
NXX	Temporary storage for altitude index read from cards containing concentration data.
N1	Storage space used for sequence numbers of cards read in or punched out at a given altitude.
N2	
N3	

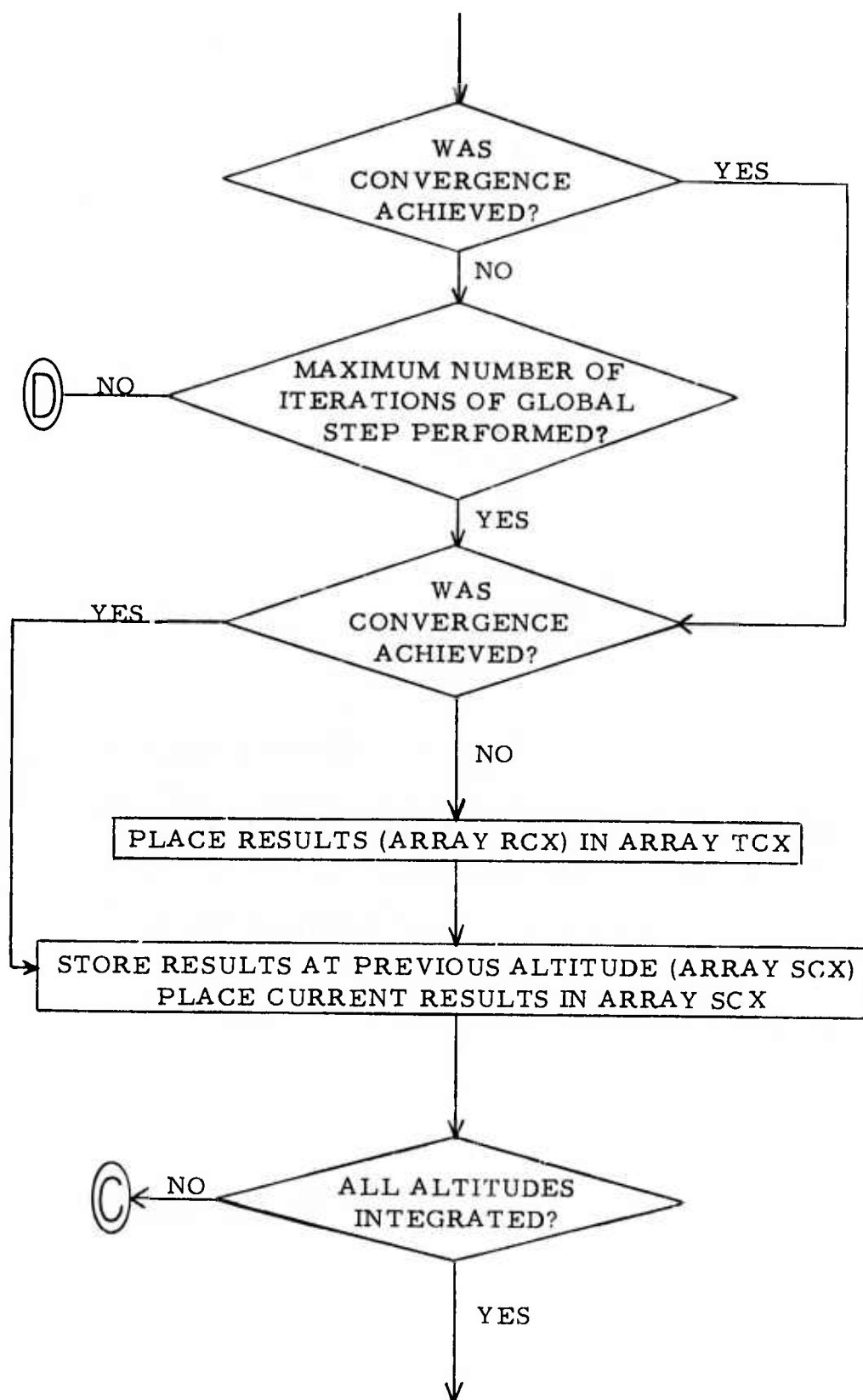
Flow Chart for Chemistry Program



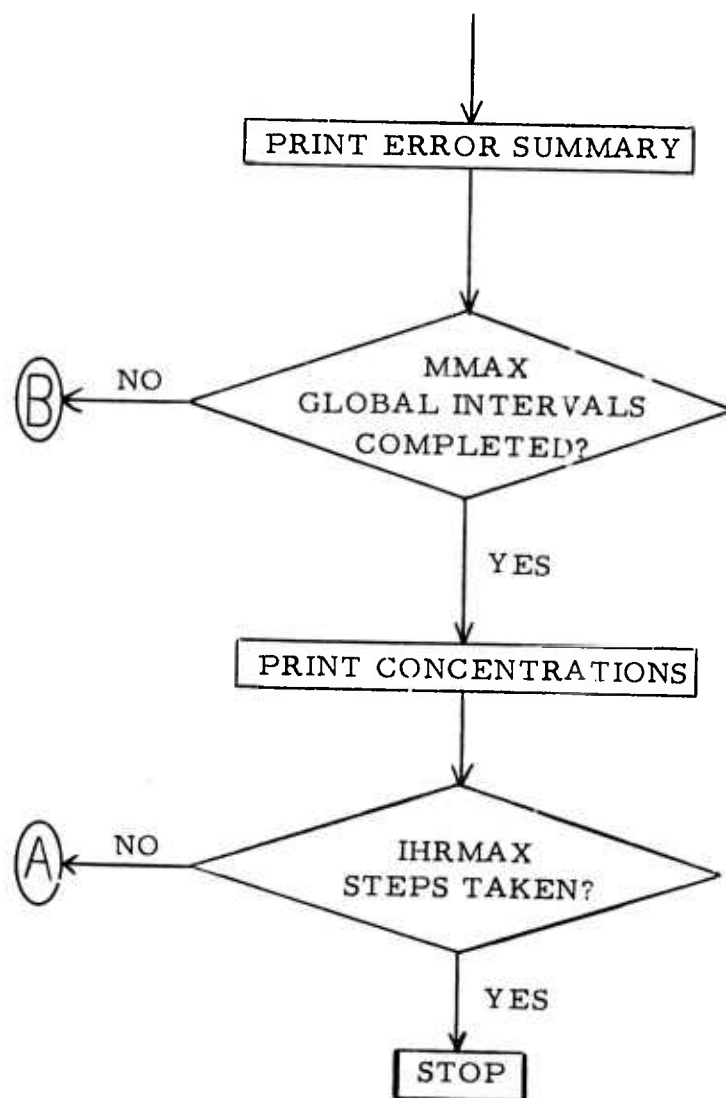
Flow Chart for Chemistry Program (continued)



Flow Chart for Chemistry Program (continued)



Flow Chart for Chemistry Program (continued)



1	(TCX(4),T03),	(TCX(5),T0H),	(TCX(6),TH),	(TCX(7),TH2C),	SNAP 370
2	(TCX(8),THC2),	(TCX(9),TH202),	(TCX(10),TH2),	(TCX(11),TCH4),	SNAP 380
3	(TCX(12),TC02),	(TCX(13),TC0),	(TCX(14),T01C),	(TCX(15),TN),	SNAP 390
4	(TCX(16),TN0),	(TCX(17),TN02),	(TCX(18),TN2C),	(TCX(19),TN2C)	SNAP 400

C

C

DATA TST /500*0.0/

DATA TINO /50*10.0,20.0,40.0,80.0,1.6E2,3.2E2,6.5E2,30*1.0E3,

1	1.5E3,2.0E3,2.5E3,3.0E3,3.5E3,4.0E3,4.5E3,5.0E3,5.5E3,6.0E3,	SNAP 410
2	1.1E4,1.6E4,2.1E4,2.6E4,3.2E4,3.5E4,4.1E4,4.3E4,4.7E4,	SNAP 420
3	395*5.0E4/	SNAP 430

DATA TETOT /50*10.0,20.0,40.0,80.0,1.6E2,3.2E2,6.5E2,26*1.0E3,

1	1.1E3,1.2E3,1.4E3,1.5E3,2.4E3,3.3E3,4.2E3,5.1E3,6.0E3,6.8E3,	SNAP 440
2	7.6E3,8.4E3,9.2E3,1.0E4,1.9E4,2.8E4,3.7E4,4.6E4,5.5E4,6.4E4,	SNAP 450
3	7.3E4,8.2E4,9.1E4,396*1.0E5/	SNAP 460

DATA TIO /91*0.0,0.1,0.2,0.3,0.4,0.5,0.7,1.0,1.5,2.5,5.0,

1	10.0,15.0,20.0,25.0,30.0,35.0,40.0,50.0,60.0,80.0,120.0,	SNAP 470
2	120.0,140.0,160.0,180.0,220.0,300.0,400.0,500.0,600.0,	SNAP 480
3	700.0,750.0,800.0,850.0,900.0,1.0E3,1.2E3,1.4E3,1.6E3,	SNAP 490
4	1.8E3,2.0E3,2.2E3,2.4E3,2.7E3,3.0E3,3.5E3,4.0E3,4.5E3,	SNAP 500
5	5.0E3,5.5E3,6.0E3,7.0E3,8.0E3,9.0E3,1.1E4,1.2E4,	SNAP 510
6	1.3E4,1.4E4,1.5E4,1.8E4,2.1E4,2.4E4,2.7E4,3.1E4,3.3E4,	SNAP 520
7	3.6E4,3.9E4,4.2E4,341*4.5E4/	SNAP 530

DATA TIO2 /81*0.0,100.0,200.0,300.0,400.0,600.0,900.0,

1	1.2E3,1.6E3,2.0E3,2.5E3,2.8E3,3.1E3,3.4E3,3.7E3,4.0E3,	SNAP 540
2	5.0E3,7.0E3,1.0E4,1.5E4,2.0E4,2.3E4,2.6E4,2.9E4,3.2E4,	SNAP 550
3	3.5E4,3.8E4,4.1E4,4.4E4,4.7E4,391*5.0E4/	SNAP 560

C

DATA LALT,LTIME,LCHI,LCOLO2,LCOLN2,LCOL03,LJ02,LJ03,LQCOHA,

1	LQCOHB,LDZCHA,LDZCHB,LML /6H	ALT,6H TIME ,6H	CHI ,6H	COLO2,	SNAP 570
2	6H COLN2,6H COLO3,6H	J02 ,6H	J03 ,6HQA(OH),	6HCB(CH),	SNAP 580
3	6HIB(OH),6H	ML/			SNAP 590

C

DATA AMWT / 28.0134, 31.9988, 15.9994, 47.9982, 17.0074,

1	1.00797, 18.0153, 33.0067, 34.0147, 2.01594, 16.0430, 44.0099,	SNAP 600
2	28.0105, 15.9994, 14.0067, 30.0061, 46.0055, 44.0128, 14.0067,	SNAP 610

```

3 39.9480, 30*0.0 /
C
DATA EDCOE / 51*1.0E5,1.09E5,1.202E5,1.318E5,1.445E5,1.585E5,
1 1.738E5,1.905E5,2.085E5,2.291E5,2.512E5,2.754E5,3.02E5,3.31E5,
2 3.63E5,3.98E5,4.36E5,4.79E5,5.25E5,5.75E5,6.31E5,6.92E5,7.59E5,
3 8.32E5,9.12E5,1.0E6,1.096E6,1.202E6,1.318E6,1.445E6,1.585E6,
4 1.738E6,1.905E6,2.085E6,2.291E6,2.512E6,2.754E6,3.02E6,3.31E6,
5 3.63E6,3.98E6,4.36E6,4.78E6,5.25E6,5.75E6,6.31E6,6.92E6,7.59E6,
6 8.32E6,9.12E6,1.0E7,1.096E7,1.20E7,1.24E7,1.27E7,1.24E7,
7 1.18E7,1.05E7,8.20E6,3.162E6,1.00E6,3.162E5,1.00E5,3.162E4,
8 1.00E4,3.162E3,1.00E3,3.162E2,1.00E2,3.162E1,1.00E1,3.80*1.0/
DATA EDCF /12*1.0E5,7.943E4,6.310E4,5.012E4,3.981E4,3.162E4,
1 2.512E4,1.995E4,1.585E4,1.259E4,11*1.0E4,1.259E4,1.585E4,
2 1.995E4,2.512E4,3.162E4,3.981E4,5.012E4,6.310E4,7.943E4/
C
DATA LSP /6H N2 ,6H O2 ,6H O(3P),6H O3 ,6H CH ,6H H ,
1 6H H2O ,6H H2O2 ,6H H2 ,6H CH4 ,6H CC2 ,6H CO ,
2 6H O(1D),6H N(4S),6H NO ,6H NO2 ,6H N2O ,6H N(2D),
3 6*6H /
C
DATA TFMT /10H(/5X,5HSTA,10HRT,6X,3HEN,10HD,7X,5HTCT,
1 10HAL,6X,5HTI,10HMES/1X,3F1,5H0.3//)
C
STATEMENT FUNCTION TC CONVERT DEGREES TO RADIAN
RAD(DEG) = 1.7453292519943E-2*DEG
C
STATEMENT FUNCTION TC COMPLETE 1.0 - EXP(-X)
EXPM(X) = (((0.008333*X - 0.04166667)*X + 0.16666666667)*X
1 - 0.5)*X + 1.0)*X
C
EDDY DIFFUSION COEFFICIENTS ARE STORED IN ARRAY EDCCEF
KINETIC TEMPERATURES ARE STORED IN ARRAY TEMPK
NUMBER DENSITIES FOR ALL ALTITUDES AND SPECIES ARE
STORED IN ARRAY CONSP
C

```


KH20 = 7
 KHC2 = 8
 KH202 = 9
 KH2 = 10
 KCH4 = 11
 KC02 = 12
 KCO = 13
 KC10 = 14
 KN = 15
 KNC = 16
 KNC2 = 17
 KN20 = 18
 KN2C = 19

C

READ (5,21) ICENT, IDNT
 WRITE (4,21) ICENT, IDNT
 WRITE (6,20) ICENT, NPAGE
 NPAGE = NPAGE + 1

C

PRINT INPUT PARAMETERS

C

C

C

C

C

WRITE (6,21) ICENT, IDNT
 READ (5,15) CTHETA, CARD
 WRITE (6,15) CTHETA, CARD
 WRITE (4,15) CTHETA, CARD
 READ (5,15) CPHI, CARD
 WRITE (6,15) OPHI, CARD
 WRITE (4,15) CPHI, CARD
 READ (5,15) SCLDEC, CARD
 WRITE (6,15) SCLDEC, CARD
 WRITE (4,15) SCLDEC, CARD
 READ (5,15) GREF, CARD
 WRITE (6,15) GREF, CARD
 WRITE (4,15) GREF, CARD
 READ (5,15) REFF, CARD

SNAP1450
 SNAP1460
 SNAP1470
 SNAP1480
 SNAP1490
 SNAP1500
 SNAP1510
 SNAP1520
 SNAP1530
 SNAP1540
 SNAP1550
 SNAP1560
 SNAP1570
 SNAP1580
 SNAP1590
 SNAP1600
 SNAP1610
 SNAP1620
 SNAP1630
 SNAP1640
 SNAP1650
 SNAP1660
 SNAP1670
 SNAP1680
 SNAP1690
 SNAP1700
 SNAP1710
 SNAP1720
 SNAP1730
 SNAP1740
 SNAP1750
 SNAP1760
 SNAP1770
 SNAP1780
 SNAP1790
 SNAP1800

```

WRITE (6,15) REFF,CARC
WRITE (4,15) REFF,CARC
READ (5,15) EPS,CARC
WRITE (6,15) EPS,CARC
WRITE (4,15) EPS,CARC
READ (5,16) MLMAX,CARD
WRITE (6,16) MLMAX,CARD
WRITE (4,16) MLMAX,CARD
READ (5,16) NEASE,CARD
WRITE (6,16) NEASE,CARD
WRITE (4,16) NEASE,CARD
READ (5,16) NTCF,CARC
WRITE (6,16) NTCF,CARC
WRITE (4,16) NTCF,CARC
READ (5,16) IHRMAX,CARD
WRITE (6,16) IHRMAX,CARD
WRITE (4,16) IHRMAX,CARD
READ (5,16) MMAX,CARC
WRITE (6,16) MMAX,CARC
WRITE (4,16) MMAX,CARC
READ (5,15) DLTIME,CARD
WRITE (6,15) DLTIME,CARD
WRITE (4,15) DLTIME,CARD
READ (5,15) TIME,CARC
WRITE (6,15) TIME,CARC

```

```

WRITE (6,20) IDENT,NPAGE
NPAGE = NPAGE + 1
DO 100 NALT = 1, 201
  READ (5,34) NXX,N1, (CONSP(NALT,J), J = 1, 7)
  WRITE (6,35) NXX,N1, (CONSP(NALT,J), J = 1, 7)
  IF (NXX.NE.NALT) GO TO 500
  IF (N1.NE.1) GO TO 530
  READ (5,34) NXX,N2, (CONSP(NALT,J), J = 8, 14)

```

C
C
C

SNAP1810
SNAP1820
SNAP1830
SNAP1840
SNAP1850
SNAP1860
SNAP1870
SNAP1880
SNAP1890
SNAP1900
SNAP1910
SNAP1920
SNAP1930
SNAP1940
SNAP1950
SNAP1960
SNAP1970
SNAP1980
SNAP1990
SNAP2000
SNAP2010
SNAP2020
SNAP2030
SNAP2040
SNAP2050
SNAP2060
SNAP2070
SNAP2080
SNAP2090
SNAP2100
SNAP2110
SNAP2120
SNAP2130
SNAP2140
SNAP2150
SNAP2160

SNAP2530
SNAP2540
SNAP2550
SNAP2560
SNAP2570
SNAP2580
SNAP2590
SNAP2600
SNAP2610
SNAP2620
SNAP2630
SNAP2640
SNAP2650
SNAP2660
SNAP2670
SNAP2680
SNAP2690
SNAP2700
SNAP2710
SNAP2720
SNAP2730
SNAP2740
SNAP2750
SNAP2760
SNAP2770
SNAP2780
SNAP2790
SNAP2800
SNAP2810
SNAP2820
SNAP2830
SNAP2840
SNAP2850
SNAP2860
SNAP2870
SNAP2880

```

RMWT = 0.0
SUMU = 0.0
SUM = 0.0
I = 0
CC 110 NALT = NEASE, NTOP
I = I + 1
NA = NALT - 1
NE = NALT - 2
TEMPL = TEMP
TEMP = TEMPU
SHL = SH
SH = SHU
GL = G
G = GU
RMWTL = RMWT
RMWT = RMWTU
SUML = SUM
SUM = SUMU
SUMU = 0.0
RMWTU = 0.0
GO 102 NSP = 1, 20
SUMU = SUMU + CCNSP(NALT,NSP)
RMWTU = RMWTU + AMWT(NSP)*CCNSP(NALT,NSP)
CONTINUE
RMWTU = RMWTU/SUMU
RCBS = NA
TEMPU = TKFL(ROBS)
RCTEMP(NALT) = 2.68684E19*(TEMPU/273.15)**0.75
TEMPK(NALT) = TEMPU
GU = GREF*(REFF/(REFF + RCBS))**2
SHU = 8.31432E7*TEMPU/(RMWTL*GU)
IF (I.EQ. 2) SHFACL = EXP(1.0E5/SHU)
IF (I.LE. 2) GC TO 110
IF (NALT.EQ. NTCF - 1) SHFAC = EXP(-1.0E5/SHU)
CTDZ = (TEMPU - TEMPL)*RDELZ
DKDZ = (EDCCCF(NALT) - EDCCCF(NB))*RDELZ

```

```

DHDZ = (SHU - SHL)*RDELZ
TFAC = QTOZ/TEMP
AFAC(NA) = TFAC
SFAC = (4.0 - (TEMPU + TEMPL)/TEMP)*R2DELZ + TFAC*TFAC
BFAC(NA) = SFAC
FAC = 1.0/SH + TFAC
EC = EDCOE(NA)
BTED(NA) = (SFAC + DHCZ/(SH*SH))*ED - FAC*DKDZ
CFAC(NA) = (TEMPU/GU - TEMPL/CL)*G*G*RDELZ/(8.31432E7*TEMP)
DFAC(NA) = G/(8.31432E7*TEMP)
FAC = (FAC*ED + CKCZ)*RDELZ
QJEDU(NA) = R2DELZ*ED + FAC
QJEDL(NA) = R2DELZ*ED - FAC
IF (IHR.GT. 1) GC TC 110
CONFAC = SUML*(QJEDL(NA)/QJEDU(NA) + 1.0)/((BTED(NA)/QJEDU(NA)
+ (TEMPU - TEMPL)/TEMP + 2.0*DELZ/SH)*SUM)
1 SUM = CONFAC*SUM
IF (NALT.EQ. NTCF) CON = (BTED(NA)*SUM - QJEDL(NA)*SUML)
1 / (QJEDU(NA)*SUMU)
DO 104 NSP = 1, NSPM
CCNSP(NA,NSP) = CCNSP(NA,NSP)*CONFAC
IF (NALT.EQ. NTCF) CCNSP(NTCP,NSP) = CON*CCNSP(NTCP,NSP)
104 CONTINUE
WRITE (6,6) NB,CCNSP(NA,1),CCNSP(NA,2),GL,SH,CTCZ,CKCZ,DHDZ,
1 BTED(NA),QJEDL(NA),QJEDU(NA)
WRITE (6,6) N1,RMT,TFAC,SFAC,CFAC(NA),DFAC(NA),RTEMP(NA)
WRITE (6,6) NALT,CCNC(1),CCNC(2),CCNC(4),CCNC(7),CCNC(9),CCNC(10)
C CONTINUE
110 NBASE = NBSAV
NBASE = NBASE + 1
NTOP = NTOP - 1
NMIN = NBASE - 1
CC 400 M = 1, MMAX
NTIME = (0.5*DLTIME + TIME)/60.0 + 720.1
RTIME = FLOAT(NTIME)/60.0
NTIME = 100*(NTIME/60) + MOD(NTIME,60)

```

SNAP2890
 SNAP2900
 SNAP2910
 SNAP2920
 SNAP2930
 SNAP2940
 SNAP2950
 SNAP2960
 SNAP2970
 SNAP2980
 SNAP2990
 SNAP3000
 SNAP3010
 SNAP3020
 SNAP3030
 SNAP3040
 SNAP3050
 SNAP3060
 SNAP3070
 SNAP3080
 SNAP3090
 SNAP3100
 SNAP3110
 SNAP3120
 SNAP3130
 SNAP3140
 SNAP3150
 SNAP3160
 SNAP3170
 SNAP3180
 SNAP3190
 SNAP3200
 SNAP3210
 SNAP3220
 SNAP3230
 SNAP3240

```

IF (MCD(M,NPRNT) .NE. 0) GO TO 120
WRITE (6,20) IDENT,NPAGE
NPAGE = NPAGE + 1
WRITE (6,6) NTIME,RTIME
WRITE (6,19)
C      WRITE (6,22) LALT,LTIME,LCHI,LCOLO2,LCCCLC3,LJJC2,LJ03
C      WRITE (6,22) LALT,LQCCHA,LCCCHB,LQZCHA,LQZCHB,(LSP(I),I=1,6)
C      WRITE (6,22) LML,(LSP(I),I=7,14)
WRITE (6,19)
CONTINUE
120  RFAC = ROTEMP(NMIN)
C1 = CONSP(NMIN,1)
C2 = CONSP(NMIN,2)
C3 = CONSP(NMIN,3)
CMDL(1) = RFAC/(C1/U.180 + C2/U.191 + C3/U.260)
CMDL(2) = RFAC/(C1/U.181 + C2/U.189 + C3/U.260)
CMDL(3) = RFAC/(C1/U.260 + C2/U.260 + C3/U.370)
RFAC = ROTEMP(NBASE)
C1 = CONSP(NBASE,1)
C2 = CONSP(NBASE,2)
C3 = CONSP(NBASE,3)
CMD(1) = RFAC/(C1/U.180 + C2/U.161 + C3/U.260)
CMD(2) = RFAC/(C1/U.181 + C2/U.189 + C3/U.260)
CMD(3) = RFAC/(C1/U.260 + C2/U.260 + C3/U.370)
CC 130 NSP = 1,NSPM
SCX(NSP) = CONSP(NBASE-1,NSP)
IF (NSP.LT. 4) GO TO 130
CMDL(NSP) = 0.707*CMDL(2)*SQRT(31.9988/AMWT(NSP) + 1.0)
CMC(NSP) = 0.707*CMD(2)*SQRT(31.9988/AMWT(NSP) + 1.0)
CONTINUE
130  DZCHA = 0.0
DZCHB = 0.0
CC 350 NALT = NBASE, NTOP
NPLU = NALT + 1
NMIN = NALT - 1
RFAC = ROTEMP(NPLU)

```

```

SNAP3250
SNAP3260
SNAP3270
SNAP3280
SNAP3290
SNAP3300
SNAP3310
SNAP3320
SNAP3330
SNAP3340
SNAP3350
SNAP3360
SNAP3370
SNAP3380
SNAP3390
SNAP3400
SNAP3410
SNAP3420
SNAP3430
SNAP3440
SNAP3450
SNAP3460
SNAP3470
SNAP3480
SNAP3490
SNAP3500
SNAP3510
SNAP3520
SNAP3530
SNAP3540
SNAP3550
SNAP3560
SNAP3570
SNAP3580
SNAP3590
SNAP3600

```

SNAP3610
SNAP3620
SNAP3630
SNAP3640
SNAP3650
SNAP3660
SNAP3670
SNAP3680
SNAP3690
SNAP3700
SNAP3710
SNAP3720
SNAP3730
SNAP3740
SNAP3750
SNAP3760
SNAP3770
SNAP3780
SNAP3790
SNAP3800
SNAP3810
SNAP3820
SNAP3830
SNAP3840
SNAP3850
SNAP3860
SNAP3870
SNAP3880
SNAP3890
SNAP3900
SNAP3910
SNAP3920
SNAP3930
SNAP3940
SNAP3950
SNAP3960

```

C1 = CONSP(NPLU,1)
C2 = CONSP(NPLU,2)
C3 = CONSP(NPLU,3)
CMDU(1) = RFAC/(C1/U.18J + C2/U.181 + C3/U.260)
CMDU(2) = RFAC/(C1/U.181 + C2/U.189 + C3/U.260)
CMDU(3) = RFAC/(C1/U.26U + C2/U.260 + C3/U.370)
AFACNA = AFAC(NALT)
BFACNA = BFAC(NALT)
CFACNA = CFAC(NALT)
DFACNA = DFAC(NALT)
QJEDUN = QJEDU(NALT)
QJEDLN = QJEDL(NALT)
BTEDNA = BTED(NALT)
DO 14U NSP = 1,NSPM
  CUNSPN = CONSP(NALT,NSP)
  DCX(NSP) = CONSPN
  TCX(NSP) = CONSPN
  CMDNSP = CMD(NSP)
  IF (NSP.LT. 4) GO TO 135
  CMDU(NSP) = U.7U7*CMDU(2)*SQRT(31.9988/AMWT(NSP) + 1.0)
135 CONTINUE
  FAC = AMWT(NSP)*CFACNA + AFACNA
  DUDZ = (CMDU(NSP) - CMDL(NSP))*RDELZ
  BTEMDS(NSP) = (BFACNA + AMWT(NSP)*CFACNA)*CMDNSP - FAC*CCCLZ
1 + BTEDNA
  FAC = (FAC*GMDNSP + DCDZ)*RDELZ
  QJEMD(NSP) = (R2DELZ*CMDNSP + FAC + QJEDUN)*CCNSP(NPLU,NSP)
1 + (R2DELZ*CMDNSP - FAC + QJEDLN)*CCNSP(NAPIN,NSP)
  GMDL(NSP) = CMDNSP
  CMD(NSP) = CMDU(NSP)
140 CONTINUE
  TEMP = TEMPK(NALT)
  RCBS = FLOAT(NALT - 1)
  CALL SOLLY (DTHTETA,ROES,TIME,SOLDEC,CHI,ETA)
  IF (ETA.LE. 0.0) GO TO 160
  CHISAV = 1.0

```


SNAP3970
SNAP3980
SNAP3990
SNAP4000
SNAP4010
SNAP4020
SNAP4030
SNAP4040
SNAP4050
SNAP4060
SNAP4070
SNAP4080
SNAP4090
SNAP4100
SNAP4110
SNAP4120
SNAP4130
SNAP4140
SNAP4150
SNAP4160
SNAP4170
SNAP4180
SNAP4190
SNAP4200
SNAP4210
SNAP4220
SNAP4230
SNAP4240
SNAP4250
SNAP4260
SNAP4270
SNAP4280
SNAP4290
SNAP4300
SNAP4310
SNAP4320

```

IF (CHI .GT. 1.0) GO TO 145
CHISAV = 1.0/CCS(CHI)
CHI = 0.0
145 CONTINUE
CALL COLUMN (RCES,CHI,COL,ETA)
COL(1) = CHISAV*COL(1)
COL(2) = CHISAV*COL(2)
COL(3) = CHISAV*COL(3)
COL(4) = CHISAV*COL(4)
150 CONTINUE
160 CONTINUE
CALL SUNPHI (COL,ETA,RATE)
TEMP1 = 1.0/TEMP
TEMP12 = SQRT(TEMP1)
TEMP32 = TEMP1*TEMP12
TEMP52 = TEMP1*TEMP32
FORWARD REACTIONS
REVERSE REACTIONS
REACTION 1 N + C2 = NC + C
R1 = 1.1E-14*TEMP*EXP(-3140.0*TEMP1)
S1 = 2.6E-15*TEMP*EXP(-19500.0*TEMP1)
REACTION 2 N + NO = N2 + C
R2 = 5.1E-11*EXP(-168.0*TEMP1)
S2 = 2.3E-10*EXP(-37500.0*TEMP1)
REACTION 3 NO + NO = N2 + C2
R3 = 1.3*TEMP52*EXP(-42800.0*TEMP1)
S3 = 15.2*TEMP52*EXP(-64300.0*TEMP1)
REACTION 4 O + C + M = C2 + M
R4 = 3.80E-30*TEMP1*EXP(-171.0*TEMP1)
S4 = 4.57E-5*TEMP1*EXP(-59700.0*TEMP1)
REACTION 5 N + N + M = N2 + M
R5 = 1.4E-33*EXP(-500.0*TEMP1)
S5 = 3.2E-7*TEMP12*EXP(-112000.0*TEMP1)
REACTION 6 N + N + N2 = N2 + N2
R6 = 7.3E-32*TEMP12
S6 = 7.8E-7*TEMP12*EXP(-112000.0*TEMP1)

```

C	REACTION 7	N + N + N = N2 + N	SNAP4330
	R7 =	6.25E-27*TEMP32	SNAP4340
C	S7 =	6.75E-2*TEMP32*EXP(-112000.0*TEMP)	SNAP4350
	REACTION 8	N + O + M = NC + M	SNAP4360
	R8 =	1.1E-32*SQRT(273.0*TEMP)	SNAP4370
C	S8 =	3.8E-7*TEMP12*EXP(-74500.0*TEMP)	SNAP4380
	REACTION 9	NO + O = NC2 + F-NU	SNAP4390
	R9 =	6.5E-17*TEMP/296.0	SNAP4400
	S9 =	RATE(4)	SNAP4410
C	REACTION 10	O + NO2 = NO + O2	SNAP4420
	R10 =	1.6E-11*EXP(-300.0*TEMP)	SNAP4430
	S10 =	1.0E-37	SNAP4440
C	REACTION 11	N + NO2 = N2 + O2	SNAP4450
	R11 =	2.3E-12	SNAP4460
	S11 =	1.0E-37	SNAP4470
C	REACTION 12	N + NO2 = NO + NO	SNAP4480
	R12 =	5.9E-12	SNAP4490
	S12 =	1.0E-35	SNAP4500
C	REACTION 13	NO + O + M = NC2 + M	SNAP4510
	R13 =	2.9E-33*EXP(940.0*TEMP)	SNAP4520
	S13 =	1.8E-8*EXP(-32800.0*TEMP)	SNAP4530
C	REACTION 14	NO + NC + O2 = NO2 + NC2	SNAP4540
	R14 =	6.6E-39*EXP(530.0*TEMP)	SNAP4550
	S14 =	6.6E-12*EXP(-13500.0*TEMP)	SNAP4560
C	REACTION 15	O + C = O2 + F-NU	SNAP4570
	S15 =	RATE(1)	SNAP4580
C	REACTION 16	N + O = NO + F-NU	SNAP4590
	S16 =	RATE(3)	SNAP4600
C	REACTION 21	NC + O3 = O2 + NC2	SNAP4610
	R21 =	9.5E-13*EXP(-1240.0*TEMP)	SNAP4620
	S21 =	1.0E-13*EXP(-23900.0*TEMP)	SNAP4630
	REACTION 31	O + O2 + M = C3 + M	SNAP4640
	R31 =	4.63E-35*EXP(1060.00*TEMP)	SNAP4650
	S31 =	1.65E-9*EXP(-11920.0*TEMP)	SNAP4660
	REACTION 32	C + C3 = O2 + C2	SNAP4670
	R32 =	2.00E-11*EXP(-2410.0*TEMP)	SNAP4680

S32 = 2.12E-11*EXP(-50700.0 * TEMPI)
 REACTION 33 H + O3 = OH + C2
 R33 = 2.6E-11
 S33 = 0.
 REACTION 34 C + CH = H + C2
 R34 = 2.06E-11
 S34 = 4.19E-10 * EXP(-8450.0*TEMPI)
 R35 H2 + C = CH + C2
 R35 = 1.0E-11
 R36 H2 + H = CH + CH
 R36 = 2.0E-10*EXP(-2000.0*TEMPI)
 R37 H + O2 + M = H2 + M
 R37 = 3.0E-32*(273.0*TEMPI)**1.3
 R38 OH + C3 = HC2 + O2
 R38 = 5.0E-13
 R39 H2 + O3 = CH + O2 + C2
 R39 = 1.0E-14
 R40 OH + CH = H2O + O
 R40 = 9.3E-12*EXP(-390.0*TEMPI)
 S40 = 9.3E-11*EXP(-9000.0*TEMPI)
 R41 OH + H2 = H2O + O2
 R41 = 1.0E-11
 R42 H + HC2 = H2 + C2
 R42 = 2.0E-13
 R43 O + H2 = CH + H
 R43 = 7.0E-11*EXP(-5190.0*TEMPI)
 R44 H2 + H2 = H2O2 + O2
 R44 = 1.5 E-12
 R45 OH + H2O2 = H2O + H2O
 R45 = 4.0E-13
 R46 O + H2O2 = CH + H2O
 R46 = 1.0E-15
 R47 H + H2O2 = H2 + H2O
 R47 = 1.0E-13
 R50 O(1D) + C3 = O2 + C2
 R50 = 5.0E-11

SNAP4690
 SNAP4700
 SNAP4710
 SNAP4720
 SNAP4730
 SNAP4740
 SNAP4750
 SNAP4760
 SNAP4770
 SNAP4780
 SNAP4790
 SNAP4800
 SNAP4810
 SNAP4820
 SNAP4830
 SNAP4840
 SNAP4850
 SNAP4860
 SNAP4870
 SNAP4880
 SNAP4890
 SNAP4900
 SNAP4910
 SNAP4920
 SNAP4930
 SNAP4940
 SNAP4950
 SNAP4960
 SNAP4970
 SNAP4980
 SNAP4990
 SNAP5000
 SNAP5010
 SNAP5020
 SNAP5030
 SNAP5040

```

C      R51  O(ID) + N2 = O + N2
R51 = 5.0E-11
C      R52  O(ID) + H2 = OH + H
R52 = 1.0E-11
C      R53  O(ID) + H2O = OH + OH
R53 = 3.0E-11
C      R54  O(ID) + CH4 = PRODUCTS
R54 = 1.0E-11
C      R55  CH4 + OH = H2O + CH3
R55 = 1.2E-10*EXP(-2960.0*TEMP)
C      R56  O + CH4 = CH + CH3
R56 = 3.5E-11*EXP(-4550.0*TEMP)
C      R60  CO + CH = CO2 + H
R60 = 1.0E-12*EXP(-540.0*TEMP)
C      R61  CO + C + M = CO2 + M
R61 = 1.4E-33*EXP(-1250.0*TEMP)
C      IONIC REACTION 1  O2+ + E = C + O
RI1 = 6.0E-5*TEMP
SI1 = 0.0
C      IONIC REACTION 2  N2+ + E = N + N
RI2 = 9.0E-5*TEMP
SI2 = 0.0
C      IONIC REACTION 3  N2+ + O2 = N2 + O2+
RI3 = 1.0E-10
SI3 = 0.0
C      IONIC REACTION 4  N2+ + E = N2 + H-NU
RI4 = 1.0E-16
SI4 = 1.0E-16
C      WRITE (6,19)
NA = NALT - 1
C
C      170  CONTINUE
C
C      DO 300 ML = 1, MLMAX

```

```

SNAP5050
SNAP5060
SNAP5070
SNAP5080
SNAP5090
SNAP5100
SNAP5110
SNAP5120
SNAP5130
SNAP5140
SNAP5150
SNAP5160
SNAP5170
SNAP5180
SNAP5190
SNAP5200
SNAP5210
SNAP5220
SNAP5230
SNAP5240
SNAP5250
SNAP5260
SNAP5270
SNAP5280
SNAP5290
SNAP5300
SNAP5310
SNAP5320
SNAP5330
SNAP5340
SNAP5350
SNAP5360
SNAP5370
SNAP5380
SNAP5390
SNAP5400

```

```

      MLSAVE = ML
      MMF = (MOD(ML + 1,2) + 2)*2**((ML - 1)/2)
      IF (MLMAX .EQ. 1) MMF = 1
      DO 180 NSP = 1, NSPM
        DCX(NSP) = CCNSP(NALT, NSP)
180    CCNTINUE
      DO 190 MMS = 1, MMF
        DO 190 NSP = 1, NSPM
          TCX(NSP) = DCX(NSP)
190    CCNTINUE
      DTIME = 0.5*DLTIME/FLCAT(MMF)
      ITER = 1
200    CONTINUE
      XM4 = TN2/3.0 + TC2 + 3.0*TC
      XM5 = T02 + TNO + TO
      XM8 = XM4
      XM13 = XM4 - TNC + TNC2
      XM31 = 0.39*TN2 + 0.44*TC2
      XM37 = TN2 + TC2
      XM61 = XM37 + TC
      DO 255 NSP = 1, NSPM
        DCT = DCX(NSP)
        GC TO (201, 202, 203, 204, 205, 206, 207, 208, 209, 210, 211, 212, 213, 214,
1      215, 216, 217, 218, 219, 220, 221, 222, 223, 224, 225), NSP
      C
      C      MOLECULAR NITROGEN
      C 201    CONTINUE
      RCX(KN2) = DCT
      APT = 0.0
      BIT = 0.0
      GJT = 0.0
      GC TC 251
      C
      C      MOLECULAR OXYGEN
      C 202    CONTINUE
      APT = 2.0*S32

```

SNAP5410
 SNAP5420
 SNAP5430
 SNAP5440
 SNAP5450
 SNAP5460
 SNAP5470
 SNAP5480
 SNAP5490
 SNAP5500
 SNAP5510
 SNAP5520
 SNAP5530
 SNAP5540
 SNAP5550
 SNAP5560
 SNAP5570
 SNAP5580
 SNAP5590
 SNAP5600
 SNAP5610
 SNAP5620
 SNAP5630
 SNAP5640
 SNAP5650
 SNAP5660
 SNAP5670
 SNAP5680
 SNAP5690
 SNAP5700
 SNAP5710
 SNAP5720
 SNAP5730
 SNAP5740
 SNAP5750
 SNAP5760

```

BTT = S4*XM4 + R31*XM31*T0 + (S34 + R37*XM37)*TH + RATE(1)
QJT = ((R32*T0 + R39*TH02 + R50*T01D)*2.U + RATE(5)
      + S31*XM31 + R33*TH + R38*TCH)*T03
      + (R4*XM4*T0 + R34*TCH + R35*THC2)*T0
      + (R41*TOH + R42*TH + R44*THC2)*THC2
GC TO 251

      ATOMIC OXYGEN, O(3P)
      CCNTINUE
      APT = 2.0*R4*XM4
      BTT = R31*XM31*T02 + R32*T03 + R34*TCH + R35*THC2
      + R43*TH2 + R46*TH202 + R5E*TC4 + R61*XM61*TC
      QJT = (2.0*S4*XM4 + S32*T02 + S34*TH + RATE(8))*TC2
      + (S31*XM31 + RATE(1U))*TC3 + R4U*TOH*TOH + R51*TN2*T01D
      GO TC 251

      CZONE
      CONTINUE
      APT = 0.0
      BTT = S31*XM31 + R32*T0 + R33*TH + R38*TOH + R39*THC2
      + R50*T01D + RATE(5)
      QJT = (R31*XM31*T0 + S32*T02)*T02
      GC TO 251

      HYDROXYL
      CCNTINUE
      APT = 2.0*R40
      BTT = R34*TC + R38*T03 + R41*TH02 + R45*TH202 + R60*TCO
      + R55*TC4
      QJT = (R35*TH02 + R43*TH2 + R46*TH202 + R56*TC4)*TC
      + (R52*TH2 + 2.0*R53*TH20 + F54*TC4)*T01D + R39*THC2*TC3
      + (R33*T03 + S34*T02 + 2.0*R36*TH02)*TH + 2.0E-5*RATE(5)*TH202
      + RATE(6)*TH20
      GC TO 251

      ATOMIC HYDROGEN

```

```

206      CCNTINUE
      APT = 0.0
      BTT = (S34 + R37*XM37)*T02 + (R42 + R36)*TH02 + R33*TC3
      1 + R47*TH202
      1 GJT = (R34*TOH + R43*TH2)*TC + R52*TC1D*TH2 + R60*TC*TC
      1 + RATE(6)*TH20 + RATE(7)*TC*H4
      GC TO 251
C
C      WATER VAPOR
      207      CCNTINUE
      APT = 0.0
      BTT = R53*TC1C + RATE(6)
      GJT = (R40*TC + R41*TH02 + R45*TH2C2 + R55*TC*H4)*TC
      GO TO 251
C
C      FERHYDROXYL
      208      CCNTINUE
      APT = 2.0*R44
      BTT = R35*TC + R39*TC3 + R41*TOH + (R36 + R42)*TH
      GJT = (R45*TC + R46*TO + R47*TH)*TH202 + R38*TC*TC3
      1 + R37*XM37*TH*TC2
      GO TO 251
C
C      HYDROGEN PEROXIDE
      209      CCNTINUE
      APT = 0.0
      BTT = R45*TC + R46*TC + R47*TH + 1.0E-2*RATE(5)
      GJT = R44*THC2*THC2
      GC TO 251
C
C      MOLECULAR HYDROGEN
      210      CCNTINUE
      APT = 0.0
      BTT = R43*TC + R52*TO1D
      GJT = (R42*THC2 + R47*TH202)*TH
      GC TO 251

```

```

SNAP6130
SNAP6140
SNAP6150
SNAP6160
SNAP6170
SNAP6180
SNAP6190
SNAP6200
SNAP6210
SNAP6220
SNAP6230
SNAP6240
SNAP6250
SNAP6260
SNAP6270
SNAP6280
SNAP6290
SNAP6300
SNAP6310
SNAP6320
SNAP6330
SNAP6340
SNAP6350
SNAP6360
SNAP6370
SNAP6380
SNAP6390
SNAP6400
SNAP6410
SNAP6420
SNAP6430
SNAP6440
SNAP6450
SNAP6460
SNAP6470
SNAP6480

```

```

C      C      211      METHANE
C      CONTINUE
C      APT = 0.0
C      BTT = RATE(7) + R54*T01D + R55*TOH + R56*TO
C      QJT = 0.0
C      GO TO 251

C      C      212      CARBON DIOXIDE
C      CONTINUE
C      APT = 0.0
C      BTT = RATE(2) + 1.0E-9*ETA*TI(NALT)
C      XXX12 = R60*TOH + R61*XM61*TC
C      QJT = XXX12*TC
C      GO TO 251

C      C      213      CARBON MONOXIDE
C      CONTINUE
C      APT = 0.0
C      BTT = XXX12
C      QJT = (RATE(2) + 1.0E-9*ETA*TI(NALT))*TC02
C      GO TO 251

C      C      214      ATOMIC OXYGEN, O(10)
C      CONTINUE
C      APT = 0.0
C      BTT = R50*TC3 + R51*TN2 + R52*TH2 + R53*TH20 + R54*ICH4
C      QJT = RATE(2)*TCC2 + RATE(9)*TO2 + RATE(11)*TC3
C      GO TO 251

C      C      215      ATOMIC NITROGEN, N(4S)
C      CONTINUE
C      QJT = ((S5*XM5 + S6*TN2 + S7*TN)*2.0 + S2*TO
C      1 + S11*TO2)*TN2 + (S1*TO + S8*XM8 + S12*TN + S16)*TN0
C      3 + 1.0E-14*TN2*TN2C
C      BTT = (R11 + R12)*TN02 + R8*XM8*TO + R2*TN0 + R1*TC2

```

SNAP6490
 SNAP6500
 SNAP6510
 SNAP6520
 SNAP6530
 SNAP6540
 SNAP6550
 SNAP6560
 SNAP6570
 SNAP6580
 SNAP6590
 SNAP6600
 SNAP6610
 SNAP6620
 SNAP6630
 SNAP6640
 SNAP6650
 SNAP6660
 SNAP6670
 SNAP6680
 SNAP6690
 SNAP6700
 SNAP6710
 SNAP6720
 SNAP6730
 SNAP6740
 SNAP6750
 SNAP6760
 SNAP6770
 SNAP6780
 SNAP6790
 SNAP6800
 SNAP6810
 SNAP6820
 SNAP6830
 SNAP6840

SNAP6650
 SNAP6660
 SNAP6670
 SNAP6680
 SNAP6690
 SNAP6700
 SNAP6710
 SNAP6720
 SNAP6730
 SNAP6740
 SNAP6750
 SNAP6760
 SNAP6770
 SNAP6780
 SNAP6790
 SNAP6800
 SNAP6810
 SNAP6820
 SNAP6830
 SNAP6840
 SNAP6850
 SNAP6860
 SNAP6870
 SNAP6880
 SNAP6890
 SNAP6900
 SNAP6910
 SNAP6920
 SNAP6930
 SNAP6940
 SNAP6950
 SNAP6960
 SNAP6970
 SNAP6980
 SNAP6990
 SNAP7000
 SNAP7010
 SNAP7020
 SNAP7030
 SNAP7040
 SNAP7050
 SNAP7060
 SNAP7070
 SNAP7080
 SNAP7090
 SNAP7100
 SNAP7110
 SNAP7120
 SNAP7130
 SNAP7140
 SNAP7150
 SNAP7160
 SNAP7170
 SNAP7180
 SNAP7190
 SNAP7200

APT = (R5*XM5 + R6*TN2 + R7*TN)*2.0
 GO TO 251

 C
 C
 216
 NITRIC OXIDE
 CONTINUE
 GJT = ((R12*TN + S14*TN02)*2.0 + S9 + R10*TC
 1 + S13*XM13)*TN02 + (R1*TN02 + R8*XM8*TN)*TN
 2 + (S2*TN + 2.0*S3*TN02)*TN2
 3 + 5.0E-12*TN20*TC2
 BTT = (R13*XM13 + R9 + S1)*TC + F2*TN + R21*TC3
 1 + S8*XM8 + S10*TN02 + S16
 2 + 0.1*RATE(7)
 APT = (R14*TN02 + S12 + R3)*2.0
 GO TO 251

 C
 C
 217
 NITROGEN DIOXIDE
 CONTINUE
 GJT = ((2.0*R14*TN0 + R13*XM13 + R9)*TN + R21*TC3
 1 + S12*TN0 + S10*TN02)*TN0 + S11*TN2*TN02
 BTT = (R11 + R12)*TN + S9 + R10*TN + S13*XM13
 APT = 0.0
 GO TO 251

 C
 C
 218
 NITRICUS OXIDE
 CONTINUE
 GJT = 0.0
 BTT = 0.0
 APT = 0.0
 GO TO 251

 C
 C
 219
 ATOMIC NITROGEN, N(2C)
 CONTINUE
 QJ1 = 1.5E-4*TEMPFI*ETA*TN0(NALT)*TETOT(NALT)
 BTT = 1.0E-14*TN2 + 5.0E-12*TN02
 APT = 0.0
 GO TO 251

SNAP7210
SNAP7220
SNAP7230
SNAP7240
SNAP7250
SNAP7260
SNAP7270
SNAP7280
SNAP7290
SNAP7300
SNAP7310
SNAP7320
SNAP7330
SNAP7340
SNAP7350
SNAP7360
SNAP7370
SNAP7380
SNAP7390
SNAP7400
SNAP7410
SNAP7420
SNAP7430
SNAP7440
SNAP7450
SNAP7460
SNAP7470
SNAP7480
SNAP7490
SNAP7500
SNAP7510
SNAP7520
SNAP7530
SNAP7540
SNAP7550
SNAP7560

```

C 220 CCNTINUE
    QJT = 0.0
    BTT = 0.0
    APT = 0.0
    GO TO 251

C 221 CCNTINUE
    GO TO 253
222 CCNTINUE
    GO TO 253
223 CCNTINUE
    GO TO 253
224 CCNTINUE
    GO TO 253
225 CCNTINUE
    GO TO 253
251 CCNTINUE
    BTT = BTT + BTEMQ(NSP)
    QJT = QJT + QJEMQ(NSP)
    IF (APT .LE. 0.0) GO TO 252
    FAC4AC = 4.0*APT*GJT
    BTSQ = BTT*BTT
    FACRT = FAC4AC/BTSQ
    DLT = SQRT(FAC4AC + BTSQ)
    FACOMB = DLT - BTT
    IF (FACRT .LT. 0.01) FACOMB = (((0.027344 - 0.0205*FACRT)
1 *FACRT - 0.0390625)*FACRT + 0.0625)*FACRT - 0.125)*FACRT
2 + 0.5)*FACRT*BTT
    FAC2AX = 2.0*APT*GCT
    FACB = DLT*QTIME
    FAC = EXP(AMAX1(-675.0,AMIN1(-FACB,675.0)))
    FACM = 1.0 - FAC
    IF (FACB .LT. 0.01) FACM = EXPM(FACB)
    RCX(NSP) = ((BTT + DLT)*FAC + FACOMB)*CCT + 2.0*GJT*FACM
1 /(((FAC2AX + BTT)*FACM + (FAC + 1.0)*DLT)

```

```

252      GO TO 253
      CONTINUE
      FACB = BTT*CTIME
      FAC = EXP(AMAX1(-675.0,AMIN1(-FACB,675.0)))
      FACM = 1.0 - FAC
      IF (FACB .LT. 0.01) FACM = EXPM(FACB)
      RCX(NSP) = DCT*FAC + FACM*QJT/BTT
253      CONTINUE
255      CONTINUE
      ITER = ITER + 1
      IF (ITER .GT. 2) GO TO 260
      GO 258 NSP = 1, NSPM
      TCX(NSP) = RCX(NSP)
258      CONTINUE
      DTIME = 2.0*DTIME
      IF (ITER .EG. 2) GC TC 260
260      CONTINUE
270      CONTINUE
      DO 280 NSP = 1, NSPM
      DCX(NSP) = AES(RCX(NSP))
280      CONTINUE
290      CONTINUE
      IF (MLMAX .EQ. 1) GO TO 310
      CALL ROMTST (ML, NSPM, DCX, IST, TCX, KTEST, EPS)
      IF (KTEST .EG. 0) GC TC 310
300      CONTINUE
310      CONTINUE
      ML = 100*KTEST + MLSAVE
      MLPRNT(NALT) = ML
      IF (KTEST .EQ. 0) GO TO 318
      GO 315 NSP = 1, NSPM
      TCX(NSP) = RCX(NSP)
315      CONTINUE
318      CONTINUE
      GO 320 NSP = 1, NSPM
      CCNSP(NAMIN, NSP) = SCX(NSP)

```

```

SNAP7570
SNAP7580
SNAP7590
SNAP7600
SNAP7610
SNAP7620
SNAP7630
SNAP7640
SNAP7650
SNAP7660
SNAP7670
SNAP7680
SNAP7690
SNAP7700
SNAP7710
SNAP7720
SNAP7730
SNAP7740
SNAP7750
SNAP7760
SNAP7770
SNAP7780
SNAP7790
SNAP7800
SNAP7810
SNAP7820
SNAP7830
SNAP7840
SNAP7850
SNAP7860
SNAP7870
SNAP7880
SNAP7890
SNAP7900
SNAP7910
SNAP7920

```

```

SCX(NSP) = ABS(TCX(NSP))
IF(NALT.EQ. NTCP) CONSP(NALT,NSP) = SCX(NSP)
IF (NALT.EG. NTCP)
1  CONSP(NPLU,NSP) = SCX(NSP)*EXP(-1.0E5*AMWT(NSP)*CFACNA)
320  CONTINUE
QCOHA = R33*TCX(KH)*TCX(KO3)
QCOHB = R35*TCX(KH02)*TCX(KC)
DZOHA = DZOHA + 1.0E5*QCOHA
DZOHB = DZOHB + 1.0E5*QCOHB
IF (MCD(M,NPRNT).NE. 0) GC TO 350
WRITE (6,6) NA,GCOHA,GCOHB,LZCHA,DZCHB,(TCX(I),I=1,6)
WRITE (6,6) ML,(TCX(I),I=7,16)
350  CONTINUE
IF (MCD(M,NPRNT).EQ. 0)
1  WRITE (6,30) (MLPRNT(I), I = NBASE, NTCP)
TIME = TIME + DLTIME
IF (TIME.GT. 4.32E4) TIME = TIME - 8.64E4
400  CONTINUE
TIME = TIME - 0.5*DLTIME
WRITE (4,15) TIME,CARD
NB = NBASE - 1
NT = NTOP + 1
DO 420 NALT = 1, NT
WRITE (4,34) NALT,N1,(CONSP(NALT,I), I = 1, 7)
WRITE (4,34) NALT,N2,(CONSP(NALT,I), I = 8, 14)
WRITE (4,34) NALT,N3,(CONSP(NALT,I), I = 15, 20)
420  CONTINUE
IS = 1
CQ, 440 IP = 1, 2
IF = IS + 9
NS = 1
DO 435 IX = 1, 5
NF = NS + 50
WRITE (6,20) IDENT,NPAGE
NPAGE = NPAGE + 1
WRITE (6,6) NTIME,RTIME

```

SNAP7930
 SNAP7940
 SNAP7950
 SNAP7960
 SNAP7970
 SNAP7980
 SNAP7990
 SNAP8000
 SNAP8010
 SNAP8020
 SNAP8030
 SNAP8040
 SNAP8050
 SNAP8060
 SNAP8070
 SNAP8080
 SNAP8090
 SNAP8100
 SNAP8110
 SNAP8120
 SNAP8130
 SNAP8140
 SNAP8150
 SNAP8160
 SNAP8170
 SNAP8180
 SNAP8190
 SNAP8200
 SNAP8210
 SNAP8220
 SNAP8230
 SNAP8240
 SNAP8250
 SNAP8260
 SNAP8270
 SNAP8280

```

WRITE (6,19)
WRITE (6,22) LALT, (LSF(I), I = IS, IF)
WRITE (6,19)
CC 430 NALT = NS, NF
NA = NALT - 1
WRITE (6,6) NA, (CONSP(NALT,I), I = IS, IF)
CCNTINUE
NS = NF
CCNTINUE
IS = 11
CCNTINUE
NBASE = NBASE - 1
NTOP = NTOP + 1
CALL SECOND (SECB)
SECC = SECB - SECA
WRITE (NW,TFMT) SECA,SECE,SECC
CCNTINUE
WRITE (6,20) IDENT,NPAGE
NPAGE = NPAGE + 1
CCNTINUE
WRITE (6,20) IDENT,NPAGE
NPAGE = NPAGE + 1
STOP
6 FORMAT (1X,I6,1P10E12.3)
14 FORMAT (I6,1P8E9.3)
15 FCRMAT (1X,F11.4,11A6,A2)
16 FCRMAT (1X,I11,11A6,A2)
19 FCRMAT (1X)
20 FCRMAT (50H1***** SNAP S2 CHEMISTRY ***** HARE DEVELOPMENT,
1 8H ***** ,10A6,13H ***** PAGE ,I3/)
21 FCRMAT (10A6,4A5)
22 FCRMAT (1X,A6,10(3X,A6,3X))
24 FCRMAT (I6,3X,6(1PE9.3,1P, ),3X,A3,I3,I2)
26 FCRMAT (7X,1P6E18.9)
30 FCRMAT (/ (1X,30I4))
34 FCRMAT (I4,I2,1X,1P7E10.4)
35 FCRMAT (5X,I4,I2,1X,1F7E12.4)
END

```

SNAP8290
 SNAP8300
 SNAP8310
 SNAP8320
 SNAP8330
 SNAP8340
 SNAP8350
 SNAP8360
 SNAP8370
 SNAP8380
 SNAP8390
 SNAP8400
 SNAP8410
 SNAP8420
 SNAP8430
 SNAP8440
 SNAP8450
 SNAP8460
 SNAP8470
 SNAP8480
 SNAP8490
 SNAP8500
 SNAP8510
 SNAP8520
 SNAP8530
 SNAP8540
 SNAP8550
 SNAP8560
 SNAP8570
 SNAP8580
 SNAP8590
 SNAP8600
 SNAP8610
 SNAP8620
 SNAP8630
 SNAP8640
 SNAP8650
 SNAP8660

```

C      SUBROUTINE COLUMN (HA,CHI,COL,ETA)
C      COMPUTES THE INTEGRATED COLUMNAR NUMBER DENSITIES FOR
C      COL(1)      THE COLUMNAR NUMBER DENSITY FOR 02
C      COL(2)      THE COLUMNAR NUMBER DENSITY FOR N2
C      COL(3)      THE COLUMNAR NUMBER DENSITY FOR O3
C      ALONG A PATH BEGINNING AT ALTITUDE HA AND EXTENDING TO INFINITY
C      AND MAKING AN ANGLE CHI (RADIAN) WITH RESPECT TO THE LOCAL
C      VERTICAL AT HA
C      CHI=SOLAR ZENITH ANGLE
C      COMMON CONSP(501,25)
C      DIMENSION CONC(20),COL(5),TERM(5)
C      DATA RE /6371.0/
C      DATA A23,A43 / 0.6665666666667, 1.3333333333333 /
C      RHA = RE + HA
C      RMIN = RHA*SIN(CHI)
C      IF (RMIN .LE. RE) RMIN = RE + 0.0001
C      RMINSQ = RMIN*RMIN
C      COSCHI = COS(CHI)
C      HMIN = ABS(RHA*COSCHI)
C      NPT = -HA + 1.001
C      DO 110 I = 1,4
C      TERM(I) = 0.0
C      CONTINUE
C      ISW = 1
C      R1 = RHA + 1.0
C      HSUB = HMIN
C      IF (COSCHI .GE. 0.0) GO TO 215
C      ISW = 0
C      LPT = RMIN + 1.0 - RE
C      R1 = FLOAT(LPT) + RE
C      H1 = SQRT(R1*R1 - RMINSQ)
C      HSUB = H1
C      R1 = R1 + 1.0
C      NA = LPT + 1
C      CALL CONCEN(RMIN - RE,CONC,ETA)
C      IF (MOD(NPT-LPT,2) .EQ. 0) GO TO 130

```

```

CLMN 10
CLMN 20
CLMN 30
CLMN 40
CLMN 50
CLMN 60
CLMN 70
CLMN 80
CLMN 90
CLMN 100
CLMN 110
CLMN 120
CLMN 130
CLMN 140
CLMN 150
CLMN 160
CLMN 170
CLMN 180
CLMN 190
CLMN 200
CLMN 210
CLMN 220
CLMN 230
CLMN 240
CLMN 250
CLMN 260
CLMN 270
CLMN 280
CLMN 290
CLMN 300
CLMN 310
CLMN 320
CLMN 330
CLMN 340
CLMN 350
CLMN 350

```

110

```

H13 = H1/3.0
DO 120 I = 1,4
  IF (I.EQ. 3) GO TO 120
  TERM(I) = (2.0*CONC(I) + CONSP(NA,I))*H13
120 CONTINUE
  NS = LPT + 1
  GO TO 150
130 CONTINUE
  H2 = SQRT(R1*R1 - RMINSQ) - HSUB
  HSUB = HSUB + H2
  R1 = R1 + 1.0
  H12 = 0.5*H1/H2
  H21 = 0.5*H2/H1
  HS3 = (H1 + H2)/3.0
  NB = NA + 1
  DO 140 I = 1,4
    IF (I.EQ. 3) GO TO 140
    YA = CONC(I)
    YB = CONSP(NA,I)
    YC = CONSP(NB,I)
    TERM(I) = ((YB - YC)*H12 + (YB - YA)*H21 + YA + YB + YC)*HS3
140 CONTINUE
    NS = LPT + 2
150 CONTINUE
    IF (NS.EQ. NPT) GO TO 205
    NF = NPT - 2
170 CONTINUE
    DO 200 NA = NS, NF, 2
      NB = NA + 1
      NC = NB + 1
      H1 = SQRT(R1*R1 - RMINSQ) - HSUB
      R1 = R1 + 1.0
      HSUB = HSUB + H1
      H2 = SQRT(R1*R1 - RMINSQ) - HSUB
      R1 = R1 + 1.0
      HSUB = HSUB + H2

```

```

CLMN 370
CLMN 380
CLMN 390
CLMN 400
CLMN 410
CLMN 420
CLMN 430
CLMN 440
CLMN 450
CLMN 460
CLMN 470
CLMN 480
CLMN 490
CLMN 500
CLMN 510
CLMN 520
CLMN 530
CLMN 540
CLMN 550
CLMN 560
CLMN 570
CLMN 580
CLMN 590
CLMN 600
CLMN 610
CLMN 620
CLMN 630
CLMN 640
CLMN 650
CLMN 660
CLMN 670
CLMN 680
CLMN 690
CLMN 700
CLMN 710
CLMN 720

```

CLMN 730
CLMN 740
CLMN 750
CLMN 760
CLMN 770
CLMN 780
CLMN 790
CLMN 800
CLMN 810
CLMN 820
CLMN 830
CLMN 840
CLMN 850
CLMN 860
CLMN 870
CLMN 880
CLMN 890
CLMN 900
CLMN 910
CLMN 920
CLMN 930
CLMN 940
CLMN 950
CLMN 960
CLMN 970
CLMN 980
CLMN 990
CLMN1000
CLMN1010
CLMN1020
CLMN1030
CLMN1040
CLMN1050
CLMN1060
CLMN1070
CLMN1080

```

H12 = 0.5*H1/H2
H21 = 0.5*H2/H1
HS3 = (H1 + H2)/3.0
DO 180 I = 1,4
  IF (I .EQ. 3) GO TO 180
  YA = CONSP(NA,I)
  YB = CONSP(NB,I)
  YC = CONSP(NC,I)
  TERM(I) = ((YB - YG)*H12 + (YB - YA)*H21 + YA + YB + YC)*HS3
1 + TERM(I)
180 CONTINUE
200 CONTINUE
  IF (ISW .EQ. 1) GO TO 220
205 CONTINUE
  ISW = 1
DO 210 I = 1, 4
  TERM(I) = 2.0*TERM(I)
210 CONTINUE
215 CONTINUE
  NS = NPT
  NF = MIN0(NPT + 38,198 + MOD(NPT,2))
  IF (NPT .GT. 199) GO TO 220
  IF (CHI .EQ. 0.0) GO TO 250
  GO TO 170
220 CONTINUE
  COL(1) = 1.0E5*TERM(2)
  COL(2) = 1.0E5*TERM(1)
  COL(3) = 1.0E5*TERM(4)
  RETURN
250 CONTINUE
DO 260 I = 1, 4
  TERM(I) = 0.3333333333333333*CONSP(NPT,I)
260 CONTINUE
DO 280 NA = NS, N*, 2
  NB = NA + 1
  NC = NB + 1

```


CLMN1090
CLMN1100
CLMN1110
CLMN1120
CLMN1130
CLMN1140
CLMN1150

DO 270 I = 1, 4
IF (I .EQ. 3) GO TO 270
TERM(I) = A43*CONSP(N3,I) + A23*CONSP(NC,I) + TERM(I)
270 CONTINUE
280 CONTINUE
GO TO 220
END


```

FAC = 4.0*FAC
FACB = FAC*TB
DEN = WA/(FACB - CA)
JOV = -EGVAR(DEN)
IF (JOV .NE. 0) DEN = 0.0
TIK = CA*DEN
T(I,K) = TIK
CA = FACB*DEN
WA = CA - TA
SUM = SUM + TIK
IF (TIK .EQ. 0.0) GO TO 145
GO TO 110
140 CONTINUE
IF (ABS(TIK) .GT. EPS*(1.0E5 + SUM)) KTEST = 1
145 CONTINUE
RINT(I) = SUM
150 CONTINUE
WRITE (6,7) M,KTEST,(RINT(I), I = 1, N)
RETURN
C 6 FORMAT (7X,1P6E13.9)
C 7 FORMAT (1X,2I3,1P6E13.9)
END
RTST 370
RTST 380
RTST 390
RTST 400
RTST 410
RTST 420
RTST 430
RTST 440
RTST 450
RTST 460
RTST 470
RTST 480
RTST 490
RTST 500
RTST 510
RTST 520
RTST 530
RTST 540
RTST 550
RTST 560
RTST 570
RTST 580

```

```

SUBROUTINE SOLLY (OTHEETA,DALT,TIME,SOLDEC,CHI,ETA)
DATA PI /3.1415926535398/
DATA RE /6371.0/
PID2 = PI*0.5
T = TIME
IF (T.GT. 4.32E4) T = T - 8.64E4
XCRIT = ACOS(RE/(RE + DALT)) + PID2
XMIN = XCRIT-PI/720.0
XMAX = XCRIT+PI/720.0
OLAT = PID2-OTHEETA
SINLAT = SIN(OLAT)
COSLAT = COS(OLAT)
SINDEC = SIN(SOLDEC)
COSDEC = COS(SOLDEC)
CHI = ACOS(SINLAT*SINDEC+COSLAT*COSDEC*COS(2.*PI*T/86400.))
IF (CHI.LE.XMIN) GO TO 1
IF (CHI.GE.XMAX) GO TO 2
HDR = (CHI-XMIN)*720.0/PI
ETA = 1.-(ACOS(1.-HDR)-(1.-HDR)*SQRT(2.*HDR-HDR*HDR))/PI
GO TO 3
1 ETA = 1.0
GO TO 3
2 ETA = 0.0
3 RETURN
END

```

SOLL 10
 SOLL 20
 SOLL 30
 SOLL 40
 SOLL 50
 SOLL 60
 SOLL 70
 SOLL 80
 SOLL 90
 SOLL 100
 SOLL 110
 SOLL 120
 SOLL 130
 SOLL 140
 SOLL 150
 SOLL 160
 SOLL 170
 SOLL 180
 SOLL 190
 SOLL 200
 SOLL 210
 SOLL 220
 SOLL 230
 SOLL 240
 SOLL 250

```

C
C
SUBROUTINE SUNPHI(DENSCO,ETA,RATE)
C
C   THIS SUBROUTINE COMPUTES THE PHOTODISSOCIATION RATES AT A
C   POINT IN THE ATMOSPHERE DUE TO THE SOLAR FLUX
C
C   DIMENSION PHIZ(30)
C   DIMENSION DENSCO(10)
C   DIMENSION RATE(30)
C   DIMENSION PHITOP(30)
C   DIMENSION XS(30,10)
C
C   DATA PHITOP / 4.59E03,2.62E09,2.86E09,2.00E09,2.59E09,1.30E10,
1 1.35E09,3.10E11,7.97E09,1.44E10,2.28E10,2.07E10,4.05E10,6.96E10,
2 1.15E11,2.06E11,5.52E11,1.28E12,2.57E12,5.90E12,1.56E13,6.39E13,
3 1.05E14,1.26E14,2.97E14,6.68E14,1.93E15,3.67E15,5.95E15,8.68E15/
C   DATA (XS(I),I=1,30) /1.51E-18,1.03E-18,7.91E-19,5.51E-19,
1 6.03E-19,1.13E-18,2.59E-19,1.03E-20,2.91E-19,5.84E-19,3.33E-18,
2 1.37E-17,1.40E-17,1.10E-17,6.54E-18,2.96E-18,7.10E-19,2.25E-20,
3 1.25E-22,2.50E-23,1.00E-23,7.30E-24,4.12E-24,1.00E-24,6*0.0/
C   DATA (XS(I),I=31,60) /6*0.0,1.59E-17,2.29E-17,6.20E-18,
1 1.23E-17,1.47E-17,6.78E-18,5.16E-18,3.44E-18,1.86E-18,9.36E-19,
2 8.25E-19,7.95E-19,6.14E-19,3.87E-19,4.07E-19,1.13E-18,3.88E-18,
3 8.82E-18,1.03E-17,5.22E-18,7.35E-19,3.65E-20,1.03E-21,0.0/
C   DATA (XS(I),I=61,90) /7*0.0,1.44E-17,6*0.0,2.65E-18,
1 4.23E-18,3.80E-18,1.11E-18,6.60E-20,11*0.0/
C   DATA (XS(I),I=91,120) /7*0.0,7.32E-20,6*0.0,
1 2.6E-19,8.6E-20,2.0E-20,6.7E-21,12*0.0/
C   DATA XS8CH4 /1.50E-17/
C   XS(I,1) ARE MOLECULAR OXYGEN TOTAL CROSS SECTIONS.
C   VALUES FOR I = 7, 30 ARE TAKEN FROM ACKERMAN (1970).
C   VALUES FOR I = 1,6 WILL BE REVISED LATER
C   XS(I,2) ARE OZONE CROSS SECTIONS FROM ACKERMAN (1970).
C   XS(I,3) ARE WATER VAPOR CROSS SECTIONS.
C   THE ONLY CROSS SECTION USED FOR CH4 IS XS8CH4 AT 1215.7 A.
C   RATE( 1) IS TOTAL O2 PHOTODISSOCIATION RATE
C   RATE( 2) IS TOTAL CO2 PHOTODISSOCIATION RATE
C   RATE( 3) IS TOTAL NO PHOTODISSOCIATION RATE
C   RATE( 4) IS TOTAL NO2 PHOTODISSOCIATION RATE
C   RATE( 5) IS TOTAL O3 PHOTODISSOCIATION RATE
C
C   SPHI 10
C   SPHI 20
C   SPHI 30
C   SPHI 40
C   SPHI 50
C   SPHI 60
C   SPHI 70
C   SPHI 80
C   SPHI 90
C   SPHI 100
C   SPHI 110
C   SPHI 120
C   SPHI 130
C   SPHI 140
C   SPHI 150
C   SPHI 160
C   SPHI 170
C   SPHI 180
C   SPHI 190
C   SPHI 200
C   SPHI 210
C   SPHI 220
C   SPHI 230
C   SPHI 240
C   SPHI 250
C   SPHI 260
C   SPHI 270
C   SPHI 280
C   SPHI 290
C   SPHI 300
C   SPHI 310
C   SPHI 320
C   SPHI 330
C   SPHI 340
C   SPHI 350
C   SPHI 360

```



```

120  ATEN = COLO2*XS(I,1) + COLO3*XS(I,2)
      PHIZ(I) = ETA*PHITOP(I)*EXP(-ATTEN)
      CONTINUE
      DJ1 = 0.0
      DO 130 I = 7, 17
        DJ1 = DJ1 + PHIZ(I)*XS(I,1)
130  CONTINUE
      DJ2 = 1.46E-7*ETA/((COLO2*5.71821E-19)**0.793455 + 1.0)
      DO 140 I = 21, 24
        DJ2 = DJ2 + PHIZ(I)*XS(I,1)
140  CONTINUE
      DJ3 = PHIZ(8)*XS(8,2)
      DO 150 I = 18, 27
        DJ3 = DJ3 + PHIZ(I)*XS(I,2)
150  CONTINUE
      DJ4 = PHIZ(28)*XS(28,2) + PHIZ(29)*XS(29,2)
      DJ5 = PHIZ(8)*XS(8,3)
      DO 160 I = 15, 19
        DJ5 = DJ5 + PHIZ(I)*XS(I,3)
160  CONTINUE
      DJ6 = PHIZ(8)*XS(8,4)
      DO 170 I = 15, 19
        DJ6 = DJ6 + PHIZ(I)*XS(I,4)
170  CONTINUE
      DJ7 = (PHIZ(7) + PHIZ(8))*1.0E-19
      DO 180 I = 9, 19
        DJ7 = DJ7 + 1.0E-18*PHIZ(I)
180  CONTINUE
      RATE(1) = DJ1 + DJ2
      RATE(2) = DJ6
      RATE(3) = DJ7
      RATE(4) = DJ7
      RATE(5) = DJ3 + DJ4
      RATE(6) = DJ5
      RATE(7) = XS8CH4*PHIZ(8)
      RATE(8) = RATE(1) + DJ2

```

```

SPHI 730
SPHI 740
SPHI 750
SPHI 760
SPHI 770
SPHI 780
SPHI 790
SPHI 800
SPHI 810
SPHI 820
SPHI 830
SPHI 840
SPHI 850
SPHI 860
SPHI 870
SPHI 880
SPHI 890
SPHI 900
SPHI 910
SPHI 920
SPHI 930
SPHI 940
SPHI 950
SPHI 960
SPHI 970
SPHI 980
SPHI 990
SPHI1000
SPHI1010
SPHI1020
SPHI1030
SPHI1040
SPHI1050
SPHI1060
SPHI1070
SPHI1080

```


RATE(9) = DJ1
RATE(10) = DJ4
RATE(11) = DJ3
500 CONTINUE
RETURN
END

SPHI11090
SPHI11100
SPHI11110
SPHI11120
SPHI11130
SPHI11140

